CHEMISTRY OF MATERIALS

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MARDER 1137-1147

Representative syntheses of stilbazolium salts, ^1H NMR and elemental analytical data for salts of **1[1]**, **1[2]**, **2[1]**, **2[2]**, **3**, **6**, **7**, **8**, and **9** (8 pages).

I-1147-M1

Representative Syntheses

Preparation of 4-N-methyl picolinium *p*-toluenesulfonate:

To a solution of 4-picoline (104.5 mL) in CH_2Cl_2 (300 mL) was added methyl-*p*-toluenesulfonate (100g). The solution was stirred for 12h at which time diethyl ether (300 mL) was added, affording a white crystalline solid that was isolated by filtration, washed with additional ether and dried (150g). This material was used without further purification. This procedure worked equally well for the trifluoromethanesulfonate salt, however since this reaction is considerably more exothermic, care should be taken to add the trifluoromethanesulfonate dropwise, with stirring.

Sample procedure for the synthesis of stilbazolium salts:

4-N-methylpicolinium *p*-toluenesulfonate (0.5 g) was dissolved in methanol (10 mL) and piperidine (1 mL) is added. The resulting solution developed a yellow tinge. To this solution the desired aldehyde (> 10% excess) was added. The solution was stirred at 60° C (under an Ar atmosphere when air sensitive aldehydes were employed) for 4 h, over which time the solution turned to the color of the product. The solution was cooled to ambient temperature and, in air, diethyl ether was slowly added to afford crystals which were isolated by filtration and washed with 4:1 diethyl ether:methanol until the washings are only lightly colored. The crystals were dried under vacuum.

Large scale one pot synthesis **2[1]** $CH_3C_6H_4SO_3$:

4-picoline (50 mL) and methyl-*p*-toluenesulfonate (60g) were placed in a 1L Erlenmeyer flask with 250 mL methanol and stirred at ambient temperature for 1h. The solution was then heated to 60° C for 1h and cooled to ambient temperature. Piperidine (90 mL) was added, followed by 4-anisaldehyde (90 mL). The solution was heated and

stirred at 60° C for 4 hours, over which time the solution turned deep yellow. The compound was isolated by a procedure analogous to given in the general synthesis (69g).

Conversion of trifluoromethanesulfonate salts to chloride salts by metathesis:

The trifluoromethanesulfonate salts were dissolved in roughly 200% more than the minimum amount of acetone, and a hydrated tetra-*n*-butylammonium chloride (~0.2M) solution in acetone was added dropwise with stirring, yielding a precipitate. The addition was continued until an additional drop afforded no further precipitate. The precipitate was isolated by filtration and washed with acetone and dried.

Conversion of chloride salts to tetrafluoroborate salts by metathesis.

The chloride salts were dissolved in roughly 200% more than the minimum amount of water and a saturated aqueous sodium tetrafluoroborate solution was added dropwise with stirring yielding a precipitate. The addition was continued until an additional drop afforded no precipitate. The precipitate was isolated by filtration and washed with water and dried. The resulting material was purified by recrystallization from acetone/ diethyl ether.

I-1147-173

Table ^1H NMR characterization of selected stilbazolium chromophores, in Table 1. The cation is identified the number of the aldehyde precursor in Fig. 2 of the paper. ^1H NMR spectra were recorded on Bruker WM-500 spectrometer. Chemical shifts were referenced to the solvent or to the residual protons of the solvent.

for **1[1]**: ^1H NMR ($^2H_6$-acetone), δ, 8.70 (d, J = 6.5 Hz, 2H), 8.08 (d, J = 6.7 Hz, 2H), 7.93 (d, J = 16.1 Hz, 1H), 7.61 (d, J = 8.6 Hz, 2H), 7.16 (d, J = 16.0 Hz, 1H), 6.64 (d, J = 8.9 Hz, 2H), 4.39 (s, 3H), 3.38 (s, 6H).

for **1[2]**: (^2H-chloroform), δ, 8.45 (d, J = 7.3 Hz, 2H), 7.68 (d, J = 6.7 Hz, 2H), 7.47 (dd, J = 15.3, 11.0 Hz, 1H,), 7.41 (d, J = 8.2 Hz, 2H), 6.98 (d, J = 15.3 Hz, 1H), 6.80 (dd, J = 15.0, 11.0 Hz 1H), 6.66 (d, J = 9.1 Hz, 2H), 6.47 (d, J = 15.3 Hz, 1H), 4.28 (s, 3H), 3.02 (s, 6H).

for **2[1]**: ($^2H_6$-acetone), δ, 8.87 (d, J = 6.4 Hz, 2H), 8.34 (d, J = 6.4 Hz, 2H), 8.10 (d, J = 16.5 Hz, 1H), 7.84 (d, J = 8.5 Hz, 2H), 7.49 (d, J = 16.6 Hz, 1H), 7.05 (d, J = 8.1 Hz, 2H), 4.58 (s, 3H), 3.97 (s, 3H).

for **2[2]**: (^2H-chloroform), δ, 8.82 (d, J = 6.4 Hz, 2H), 8.14 (d, J = 6.1 Hz, 2H), 7.82 (dd, J = 15.3, 8.6 Hz, 1H), 7.56 (d, J = 8.2 Hz, 2H), 7.12 (overlapping multiplets, 2H), 6.97 (d, J = 8.0 Hz, 2H), 6.89 (d, J = 15.5, Hz, 1H), 4.45 (s, 3H), 3.83 (s, 3H).

for **3**: ($^2H_6$-acetone), δ, 8.82 (d, J = 6.5 Hz, 2H), 8.18 (d, J = 6.5 Hz, 2H), 8.11 (d, J = 16.7 Hz, 1H), 7.72(d, J = 8.5 Hz, 1H), 7.44 (d, J = 16.4 Hz, 1H), 6.66 (m, 2H), 4.46 (s, 3H), 3.97, 3.89 (each, s, 3H).

for **6**: ($^2H_6$-acetone), δ, 8.70 (d, J = 6.5 Hz, 2H), 8.08 (d, J = 6.7 Hz, 2H), 7.93 (d, J = 16.1 Hz, 1H), 7.61 (d, J = 8.6 Hz, 2H), 7.16 (d, J = 16.0 Hz, 1H), 6.64 (d, J = 8.9 Hz, 2H,), 4.39 (s, 3H), 3.38 (m, 4H), 2.04 (m, 4H).

for **7**: ($^2H_6$-acetone), δ, 8.90 (d, J = 6.4 Hz, 2H), 8.27 (d, J = 6.5 Hz, 2H), 8.00 (d, J = 16.2 Hz, 1H), 7.71 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 16.2 Hz, 1H), 7.35 (d, J = 8.0 Hz, 2H), 4.49 (s, 3H), 2.54 (s, 3H).

for **8** ($^2H_6$-acetone), δ, 9.00 (d, J = 6.6 Hz, 2H), 8.30 (d, J = 6.7 Hz, 2H), 8.00 (d, J = 16.5 Hz, 1H), 7.72 (d, J = 8.5 Hz, 2H), 7.67 (d, J = 8.5 Hz, 2H), 7.60 (d, J = 16.4 Hz, 1H), 4.50 (s, 3H).

for **9**: ($^2H_6$-acetone), δ, 9.22 (d, J = 16.1 Hz, 1H), 9.02 (d, J = 6.8 Hz, 2H), 8.84 (d, J = 9.3 Hz, 1H), 8.64 (d, J = 8.2 Hz, 1H), 8.59 (d, J = 6.9 Hz, 2H), 8.38 (d, J = 7.4 Hz, 1H), 8.37 (d, J = 8.0 Hz, 2H), 8.34 (d, J = 9.3 Hz, 1H), 8.29 (d, J = 8.8 Hz, 1H), 8.22 (d, J = 8.9 Hz, 1H), 8.13 (t, J = 7.5 Hz, 1H), 7.88 (d, J = 16.0 Hz, 1H), 4.57(s, 3H).

I-1147-MS

Elemental analyses of selected stilbazolium compounds reported in Table 1 of the paper. The cation is identified the number of the aldehyde precursor in Fig. 2. of the paper, followed by the counterion of interest and then molecular formula is given. At the right the percentages for carbon, hydrogen and nitrogen is given; for each salt, the upper value (to the right of the molecular formula) is the expected value and immediately below that is the experimentally determined value. Elemental analyses were performed by the California Institute of Technology Analytical Facility.

Compound and formula	%C	%H	%N
for **1[1]**			
$CF_3SO_3^-$: Calcd for $C_{17}H_{19}F_3N_2O_3S$:	52.57	4.93	7.21
	52.59	5.00	7.24
$CH_3C_6H_4SO_3^-$:Calcd for $C_{23}H_{26}N_2O_3S$:	67.29	6.38	6.82
	67.51	6.46	6.70
Cl: Calcd for $C_{16}H_{19}N_2Cl$:	69.93	6.97	10.19
	62.94	7.16	9.31
for **1[2]**:			
$CF_3SO_3^-$: Calcd for $C_{19}H_{21}F_3N_2O_3S$:	55.06	5.11	6.76
	55.32	5.09	6.73
BF_4: Calcd for $C_{18}H_{21}BF_4N_2$:	61.37	6.01	7.95
	61.11	6.05	7.89
$CH_3C_6H_4SO_3^-$:Calcd for $C_{25}H_{28}N_2O_3S$:	68.78	6.46	6.42
	68.58	6.44	6.35
Cl: Calcd for $C_{18}H_{21}ClN_2$:	71.87	7.04	9.31
	65.00	6.93	8.39
for **2[1]**			
$CF_3SO_3^-$:Calcd for $C_{16}H_{16}F_3NO_4S$:	51.20	4.30	3.73
	52.54	4.23	3.54
BF_4: Calcd for $C_{15}H_{16}BF_4NO$:	57.54	5.15	4.47

	57.31	5.16	4.48
$CH_3C_6H_4SO_3^-$:Calcd for $C_{22}H_{23}NO_4S$:	66.48	5.83	3.52
	66.53	5.93	3.51
Cl: Calcd for $C_{15}H_{16}ClNO$:	68.83	6.16	5.35
	65.00	6.46	5.20
Cl: Calcd for $C_{15}H_{16}ClN{\cdot}H_2O$:	64.40	6.48	5.09
	65.00	6.46	5.20
for **2[2]**:			
$CF_3SO_3^-$: Calcd for $C_{18}H_{18}F_3NO_4S$:	53.87	4.52;	3.49
	53.73	4.56	3.39
$CH_3C_6H_4SO_3^-$ Calcd for $C_{24}H_{25}NO_4S$:	68.06	5.95	3.31
	67.91	6.01	3.39
Cl: Calcd for $C_{17}H_{18}ClNO$:	70.95	6.30	4.87
	67.01	6.39	4.65
for **3**:			
$CF_3SO_3^-$: Calcd for $C_{17}H_{18}F_3NO_5S$:	50.37	4.48	3.46
	50.25	4.41	3.33.
BF_4: Calcd for $C_{16}H_{18}BF_4NO_2$:	56.01	5.29	4.08
	55.67	5.27	4.09
Cl: Calcd for $C_{16}H_{18}ClNO_2$:	65.86	6.22	4.89
	60.44	6.40	4.49
for **6**:			
$CF_3SO_3^-$:Calcd for $C_{19}H_{21}F_3N_2O_3S$:	55.06	5.11	6.76
	54.73	5.09	6.64
BF_4: Calcd for $C_{25}H_{28}N_2SO_3$:	61.39	6.01	7.95
	60.97	6.05	7.96
$CH_3C_6H_4SO_3^-$:Calcd for $C_{18}H_{21}BF_4N_2$	68.78	6.46	6.42
	69.38	6.62	6.53

Cl: Calcd for $C_{18}H_{21}ClN_2$:	71.87	7.04	9.31
	64.19	7.01	8.35
for **7**:			
$CF_3SO_3^-$:Calcd for $C_{16}H_{16}F_3NO_3S_2$:	49.10	4.12	3.58
	49.04	4.06	3.46
BF_4: Calcd for:$C_{15}H_{16}BF_4NS$:	54.73	4.90	4.26
	54.72	4.94	4.51
$CH_3C_6H_4SO_3^-$:Calcd for $C_{22}H_{23}F_3NO_3S_2$:	63.90	5.61	3.39
	63.89	5.63	3.41
Cl: Calcd for $C_{15}H_{16}ClNS$:	64.85	5.81	5.04
	61.58	5.92	4.87
for **8**			
$CF_3SO_3^-$: Calcd for $C_{15}H_{13}BrF_3NO_3S$:	42.47	3.09	3.30
	42.49	3.15	3.33
BF_4: Calcd for $C_{14}H_{13}BBrF_4N$:	46.46	3.62	3.87
	45.86	3.58	3.87
$CH_3C_6H_4SO_3^-$:Calcd for $C_{21}H_{20}BrNO_3S$:	56.51	4.52	3.14
	56.49	4.62	3.12
Cl: Calcd for $C_{14}H_{13}BrCl$:	54.13	4.22	4.51
	47.09	4.45	3.95
for **9**:			
$CF_3SO_3^-$: Calcd for $C_{25}H_{18}F_3NO_3S$:	63.89	3.86	2.98
	63.90	3.61	2.96
$CH_3C_6H_4SO_3^-$: Calcd for $C_{31}H_{25}NO_3S$:	75.74	5.13	2.85
	75.24	5.27	2.89

I-1147-M8

Experimental details of data collection, ORTEP drawings of the cations **1[1]** $CH_3C_6H_4SO_3$ (referred to as **tosylate**), **2[1]** $CH_3C_6H_4SO_3$ (referred to as **tosylate**), **8** $Cl(H_2O)_4$ and **2[1]**$Cl(H_2O)_4$, with atom numbering, tables of crystal data, final parameters of all the atoms and complete distances and angles, observed and calculated structures factors (63 pages).

Experimental Details

A. General

All data were collected at room temperature on a CAD-4 diffractometer equipped with graphite–monochromated molybdenum radiation (λ = 0.71073 Å). Data were corrected for decay, if observed, and merged. Structures were solved by MULTAN plus structure factor–difference Fourier cycles to locate all the heavy atoms. All reflections, F_o^2 positive and negative, were used in the solution and refinement of the structures; final refinement was by full matrix least squares using F_o^2 values, with weights taken as $1/\sigma^2(F_o^2)$. Variances of the individual reflections were assigned based on counting statistics plus an additional term, $(0.014\ I)^2$. Variances of merged reflections were obtained by standard propagation of error plus another additional term, $(0.014\ \bar{I})^2$. Computer programs were those of the CRYRM Crystallographic Computing System (Duchamp, 1964), MULTAN (Main, *et al.*, 1980) and ORTEP (Johnson, 1976). Scattering factors and corrections for anomalous scattering were taken from Cromer and Waber (1974) and Cromer (1974). Hydrogen atoms were positioned by calculation or, for methyl groups, at idealized positions based on difference maps calculated in their expected planes, with C–H = 0.95 Å. Hydrogen atom thermal parameters were assigned based on the equivalent isotropic displacement parameter of the bonded atom. Hydrogen atoms that were not refined were repositioned once near the conclusion of the refinement. Ordered heavy atoms were refined with anisotropic displacement parameters, disordered heavy atoms and refined hydrogen atoms with isotropic displacement parameters. A secondary extinction parameter (Larson, 1967) was included where it appeared necessary.

B. Specific Details

4′–Dimethylamino–N–methyl-4-stilbazolium Tosylate. Methyl groups C2 and C17 showed two sets of disordered hydrogen atoms which were assigned 50% occupancy; the hydrogen atoms on the other methyl groups appeared ordered. The structure consists of planar cations arranged in layers perpendicular to the z axis, with layers of tosylate anions between them. Bond distances and angles are normal. The entire cation is planar within ±0.09Å.

4′–Methoxy–N–methyl–4–stilbazolium Tosylate. In this structure the SO_3 group of the tosylate anion showed two orientations separated by about 60° around the C–S vector. A second set of oxygen atoms was introduced at fixed positions; a population parameter refined to 0.881(9) for the first set and 1–0.881 for the second set. The cation is planar within ±0.13 Å.

4′–Bromo–N–methyl–4–stilbazolium Chloride·$4H_2O$. A complete sphere of data was collected and averaged in point group *mm2*. Imaginary components $\Delta f''$ were introduced for Br and Cl and the correct polarity was clear from refining both models. This compound and the isostructural 4′–methoxy–N–methyl–4–stilbazolium chloride have an interesting two dimensional network formed by the chloride ion and the water molecules, with each chloride ion surrounded by four water molecules and each water molecule donating two hydrogen bonds, one to a chloride ion and one to another water molecule, and accepting one hydrogen bond. These assignments were confirmed by successful refinement of the coordinates and isotropic B's of the hydrogen atoms of the water molecules. The coordination about the chloride ion is distorted square planar, with angles from 84° to 100°, 169° and 170° (all esd's 3–4°). These networks are found at approximately $x = 1/4$ and $x = 3/4$, with the cations arranged in layers between them. The Br – N1 vector is nearly perpendicular to b and makes an angle of 17° with c. The plane of the molecule is roughly parallel to the ac plane and the molecules are stacked along b, with π–π interactions of half the b axis distance, or 3.54 Å.

4′–Methoxy–N–methyl–4–stilbazolium Chloride·$4H_2O$. This compound is isostructural with the preceeding one. The distances and angles are normal.

I-1147-M11

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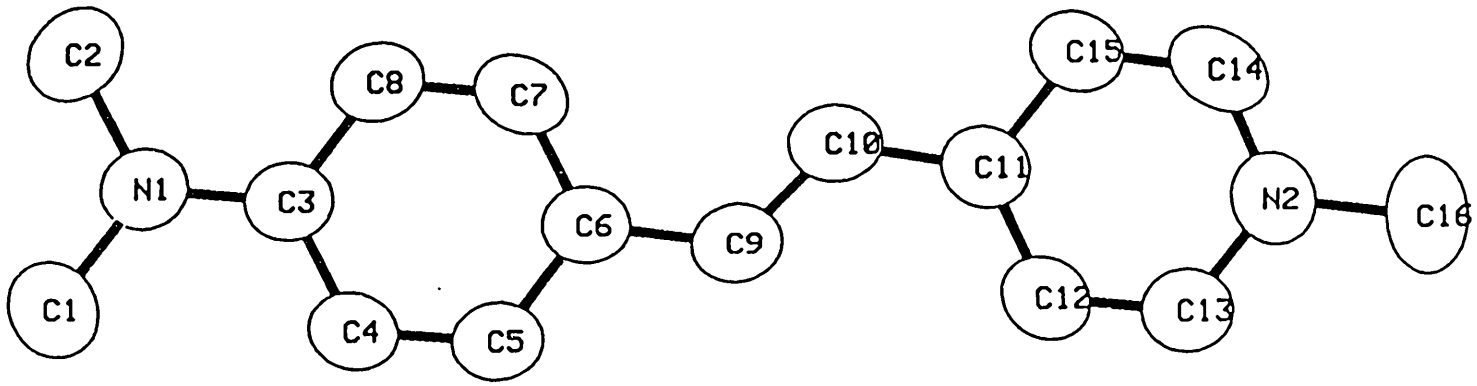

Labelled drawing of the cation of 4′–dimethylamino–N–methyl–4–stilbazolium tosylate with 70% probability ellipsoids. Hydrogen atoms are not shown.

Table S2A. Final Refined Parameters for
4'-Dimethylamino-N-methyl-4-stilbazolium Tosylate.

I-1147-M13

x, y, z and $U_{eq}{}^{a} \times 10^{4}$

Atom	x	y	z	U_{eq} or B
N 1	11012(3)	1395(3)	3301(2)	552(7)
C 1	11700(3)	1572(3)	2624(2)	606(9)
C 2	11659(3)	1767(3)	3990(2)	593(8)
C 3	9775(3)	959(3)	3275(2)	425(7)
C 4	9148(3)	640(3)	2598(2)	461(7)
C 5	7904(3)	207(3)	2586(2)	457(7)
C 6	7206(3)	68(2)	3231(2)	421(7)
C 7	7840(3)	388(3)	3908(2)	510(8)
C 8	9088(3)	815(3)	3934(2)	498(8)
C 9	5895(3)	−382(2)	3175(2)	445(7)
C10	5082(3)	−503(3)	3731(2)	456(7)
C11	3787(3)	−982(3)	3649(2)	412(7)
C12	3236(3)	−1394(3)	2974(2)	470(7)
C13	2009(3)	−1816(3)	2947(2)	477(7)
C14	1802(3)	−1484(3)	4220(2)	525(8)
C15	3030(3)	−1048(3)	4273(2)	499(8)
C16	−43(3)	−2303(3)	3506(2)	631(9)
N 2	1295(2)	−1864(2)	3560(1)	460(6)
C17	−1233(4)	2250(4)	6065(3)	893(13)
C18	215(4)	2181(3)	5996(2)	611(10)
C19	839(4)	1097(3)	5998(2)	582(9)
C20	2171(3)	1026(3)	5949(2)	497(8)
C21	2905(3)	2045(3)	5874(1)	425(8)
C22	2278(4)	3122(3)	5858(2)	550(8)

Table S2A. (Cont.)

C23	954(4)	3192(3)	5926(2)	617(9)
S	4611	1926(.7)	5789	500(2)
O 1	5096(2)	3120(2)	5745(2)	738(7)
O 2	5065(2)	1315(3)	6458(1)	727(7)
O 3	4785(3)	1255(2)	5121(1)	767(7)

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[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij} (a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

*Isotropic displacement parameter, B

Table S2B. Assigned Parameters for
4'-Dimethylamino-N-methyl-4-stilbazolium Tosylate.

I-1147-m15

Atom	x	y	z	B
	x, y and $z \times 10^4$			
H 1A	11195	2023	2260	5.8
H 1B	11891	816	2390	5.8
H 1C	12502	1971	2720	5.8
H 2A	12566	1804	3949	5.7*
H 2B	11470	1226	4396	5.7*
H 2C	11351	2540	4142	5.7*
H 2D	12176	2451	3921	5.7*
H 2E	12188	1149	4204	5.7*
H 2F	11022	1970	4363	5.7*
H16A	−650	−1673	3498	5.8
H16B	−206	−2800	3938	5.8
H16C	−181	−2780	3067	5.8
H17A	−1542	3037	6030	8.6*
H17B	−1490	1917	6537	8.6*
H17C	−1656	1786	5671	8.6*
H17D	−1484	2892	6371	8.6*
H17E	−1551	1523	6288	8.6*
H17F	−1653	2324	5580	8.6*
H 4	9581	728	2143	4.5
H 5	7513	−7	2117	4.4
H 7	7396	314	4360	5.0
H 8	9495	1016	4403	4.7
H 9	5587	−608	2689	4.3
H10	5379	−262	4217	4.5
H12	3719	−1376	2533	4.6
H13	1639	−2090	2484	4.6
H14	1295	−1508	4650	5.0
H15	3380	−802	4746	4.8
H19	345	393	6035	5.6
H20	2570	274	5966	4.7
H22	2755	3825	5798	5.2
H23	541	3934	5920	5.9

* Half-populated Site.

Table S2C. Anisotropic Displacement Parameters for 4'-Dimethylamino-N-methyl-4-stilbazolium Tosylate.

I-1147-M16

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N 1	533(16)	723(17)	400(14)	−155(14)	2(12)	−1(13)
C 1	543(21)	741(23)	539(19)	−89(16)	68(15)	67(17)
C 2	594(20)	676(22)	500(19)	−100(17)	−92(15)	31(16)
C 3	486(18)	405(16)	383(16)	3(14)	7(13)	−12(13)
C 4	502(19)	519(18)	366(16)	−1(15)	61(13)	−24(14)
C 5	509(19)	484(18)	376(16)	12(14)	5(14)	−37(13)
C 6	474(18)	401(14)	388(16)	29(14)	29(13)	−36(14)
C 7	577(21)	578(20)	382(16)	−24(16)	107(15)	−10(14)
C 8	554(20)	556(20)	381(17)	−56(15)	−22(14)	−26(14)
C 9	498(18)	421(17)	414(17)	21(13)	3(14)	−45(13)
C10	538(20)	446(17)	383(16)	29(14)	20(15)	−63(13)
C11	481(18)	345(15)	414(16)	40(13)	50(13)	5(13)
C12	501(19)	492(18)	423(17)	−7(15)	88(14)	−3(14)
C13	531(19)	494(17)	406(17)	−13(15)	7(14)	17(14)
C14	622(21)	546(19)	418(18)	31(16)	160(15)	46(14)
C15	553(20)	571(19)	377(17)	−11(16)	74(14)	−14(14)
C16	456(19)	592(21)	847(27)	−82(15)	47(18)	98(18)
N 2	452(15)	415(14)	514(15)	3(11)	48(11)	64(12)
C17	735(30)	1169(36)	783(30)	134(26)	128(23)	211(26)
C18	706(24)	732(26)	398(18)	41(19)	45(15)	66(16)
C19	692(23)	632(22)	427(18)	−119(18)	80(16)	40(16)
C20	718(24)	415(18)	365(16)	17(16)	96(15)	31(13)
C21	593(19)	454(17)	227(14)	6(15)	16(13)	−14(12)
C22	722(24)	490(19)	436(18)	−13(17)	6(15)	−41(16)
C23	745(25)	590(22)	514(20)	172(19)	16(17)	−19(17)
S	639(5)	537(5)	329(4)	−5(4)	85(3)	−32(4)
O 1	779(18)	581(15)	871(18)	−146(13)	261(14)	−36(14)
O 2	660(16)	1027(19)	494(14)	93(14)	27(11)	198(13)
O 3	874(18)	904(18)	531(15)	69(14)	119(13)	−275(13)

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table S2D. Complete Distances and Angles for 4'-Dimethylamino-N-methyl-4-stilbazolium Tosylate.

I-1147-m17

	Distance(Å)		Distance(Å)
N 1 -C 1	1.444(4)	C17 -H17F	0.961(4)
N 1 -C 2	1.443(4)	C18 -C19	1.388(5)
N 1 -C 3	1.373(4)	C18 -C23	1.385(5)
C 1 -H 1A	0.966(3)	C19 -C20	1.388(5)
C 1 -H 1B	0.976(3)	C19 -H19	0.952(3)
C 1 -H 1C	0.956(3)	C20 -C21	1.391(4)
C 2 -H 2A	0.947(3)	C20 -H20	0.947(3)
C 2 -H 2B	0.976(3)	C21 -C22	1.383(4)
C 2 -H 2C	0.974(3)	C21 -S	1.786(3)
C 2 -H 2D	0.953(3)	C22 -C23	1.384(5)
C 2 -H 2E	0.959(3)	C22 -H22	0.945(3)
C 2 -H 2F	0.984(3)	C23 -H23	0.943(4)
C 3 -C 4	1.400(4)	S -O 1	1.446(3)
C 3 -C 8	1.411(4)	S -O 2	1.445(3)
C 4 -C 5	1.380(4)	S -O 3	1.434(3)
C 4 -H 4	0.950(3)		
C 5 -C 6	1.395(4)		
C 5 -H 5	0.948(3)		
C 6 -C 7	1.401(4)		
C 6 -C 9	1.451(4)		
C 7 -C 8	1.380(4)		
C 7 -H 7	0.950(3)		
C 8 -H 8	0.951(3)		
C 9 -C10	1.337(4)		
C 9 -H 9	0.949(3)		
C10 -C11	1.449(4)		
C10 -H10	0.951(3)		
C11 -C12	1.396(4)		
C11 -C15	1.392(4)		
C12 -C13	1.357(4)		
C12 -H12	0.952(3)		
C13 -N 2	1.347(4)		
C13 -H13	0.952(3)		
C14 -C15	1.365(4)		
C14 -N 2	1.344(4)		
C14 -H14	0.949(3)		
C15 -H15	0.950(3)		
C16 -N 2	1.473(4)		
C16 -H16A	0.950(4)		
C16 -H16B	0.976(4)		
C16 -H16C	0.959(4)		
C17 -C18	1.513(6)		
C17 -H17A	0.948(4)		
C17 -H17B	0.971(4)		
C17 -H17C	0.970(4)		
C17 -H17D	0.951(4)		
C17 -H17E	0.977(4)		

Table S2D. (Cont.)

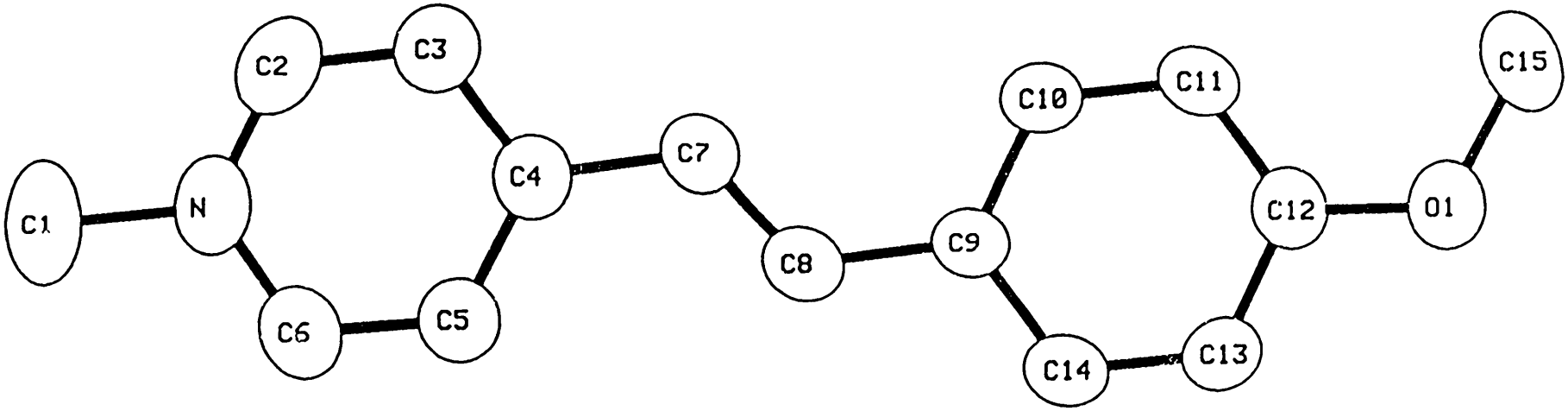
I-1147-M18

Angle(°)		Angle(°)	
C 2 -N 1 -C 1	116.6(3)	C15 -C11 -C12	116.8(3)
C 3 -N 1 -C 1	120.8(3)	C13 -C12 -C11	120.0(3)
C 3 -N 1 -C 2	122.4(3)	H12 -C12 -C11	120.0(3)
H 1A-C 1 -N 1	111.6(3)	H12 -C12 -C13	120.0(3)
H 1B-C 1 -N 1	110.7(3)	N 2 -C13 -C12	121.9(3)
H 1C-C 1 -N 1	111.7(3)	H13 -C13 -C12	119.4(3)
H 1B-C 1 -H 1A	106.7(3)	H13 -C13 -N 2	118.7(3)
H 1C-C 1 -H 1A	108.4(3)	N 2 -C14 -C15	120.6(3)
H 1C-C 1 -H 1B	107.5(3)	H14 -C14 -C15	119.8(3)
H 2A-C 2 -N 1	112.1(3)	H14 -C14 -N 2	119.6(3)
H 2B-C 2 -N 1	110.7(3)	C14 -C15 -C11	121.2(3)
H 2C-C 2 -N 1	110.8(3)	H15 -C15 -C11	119.4(3)
H 2D-C 2 -N 1	111.8(3)	H15 -C15 -C14	119.4(3)
H 2E-C 2 -N 1	111.5(3)	H16A-C16 -N 2	111.7(3)
H 2F-C 2 -N 1	110.3(3)	H16B-C16 -N 2	109.6(3)
H 2B-C 2 -H 2A	108.3(3)	H16C-C16 -N 2	110.7(3)
H 2C-C 2 -H 2A	108.6(3)	H16B-C16 -H16A	108.0(3)
H 2C-C 2 -H 2B	106.2(3)	H16C-C16 -H16A	109.4(4)
H 2E-C 2 -H 2D	109.2(3)	H16C-C16 -H16B	107.3(3)
H 2F-C 2 -H 2D	107.1(3)	C14 -N 2 -C13	119.6(3)
H 2F-C 2 -H 2E	106.8(3)	C16 -N 2 -C13	120.4(3)
C 4 -C 3 -N 1	121.5(3)	C16 -N 2 -C14	120.0(3)
C 8 -C 3 -N 1	121.0(3)	H17A-C17 -C18	112.1(4)
C 8 -C 3 -C 4	117.5(3)	H17B-C17 -C18	111.0(4)
C 5 -C 4 -C 3	120.4(3)	H17C-C17 -C18	109.5(4)
H 4 -C 4 -C 3	119.8(3)	H17D-C17 -C18	112.4(4)
H 4 -C 4 -C 5	119.8(3)	H17E-C17 -C18	110.0(4)
C 6 -C 5 -C 4	122.8(3)	H17F-C17 -C18	110.2(4)
H 5 -C 5 -C 4	118.1(3)	H17B-C17 -H17A	108.7(4)
H 5 -C 5 -C 6	119.1(3)	H17C-C17 -H17A	108.6(4)
C 7 -C 6 -C 5	116.4(3)	H17E-C17 -H17D	107.8(4)
C 9 -C 6 -C 5	119.7(3)	H17F-C17 -H17D	109.2(4)
C 9 -C 6 -C 7	123.9(3)	H17F-C17 -H17E	107.1(4)
C 8 -C 7 -C 6	121.8(3)	C19 -C18 -C17	120.6(3)
H 7 -C 7 -C 6	119.1(3)	C23 -C18 -C17	121.2(3)
H 7 -C 7 -C 8	119.1(3)	C23 -C18 -C19	118.2(3)
C 7 -C 8 -C 3	121.0(3)	C20 -C19 -C18	121.0(3)
H 8 -C 8 -C 3	119.2(3)	H19 -C19 -C18	119.3(3)
H 8 -C 8 -C 7	119.8(3)	H19 -C19 -C20	119.7(3)
C10 -C 9 -C 6	126.9(3)	C21 -C20 -C19	120.5(3)
H 9 -C 9 -C 6	116.1(3)	H20 -C20 -C19	118.9(3)
H 9 -C 9 -C10	117.0(3)	H20 -C20 -C21	120.6(3)
C11 -C10 -C 9	124.8(3)	C22 -C21 -C20	118.3(3)
H10 -C10 -C 9	117.4(3)	S -C21 -C20	119.6(2)
H10 -C10 -C11	117.7(3)	S -C21 -C22	122.1(2)
C12 -C11 -C10	124.0(3)	C23 -C22 -C21	121.0(3)
C15 -C11 -C10	119.2(3)	H22 -C22 -C21	119.8(3)

Table S2D. (Cont.)

I-1147-M19

	Angle(°)
H22 -C22 -C23	119.1(3)
C22 -C23 -C18	120.9(3)
H23 -C23 -C18	119.0(4)
H23 -C23 -C22	120.0(3)
O 1 -S -C21	106.4(1)
O 2 -S -C21	104.9(1)
O 3 -S -C21	105.5(1)
O 2 -S -O 1	113.0(1)
O 3 -S -O 1	113.2(2)
O 3 -S -O 2	112.9(2)



Labelled drawing of the cation of 4′–methoxy–N–methyl–4–stilbazolium tosylate with 50% probability ellipsoids. Hydrogen atoms are not shown.

I-1147-M21

Table S4A. Final Refined Parameters for 4'-Methoxy-N-methyl-4-stilbazolium Tosylate.

x, y, z and $U_{eq}{}^{a} \times 10^{4}$

Atom	x	y	z	U_{eq}
C1	2180(7)	16574(7)	97(3)	740(13)
N	2507(4)	14675(5)	577(2)	552(8)
C2	3843(5)	14077(7)	707(3)	630(10)
C3	4144(4)	12306(7)	1140(2)	588(9)
C4	3078(4)	11087(6)	1455(2)	473(7)
C5	1704(4)	11753(7)	1298(2)	557(8)
C6	1445(5)	13542(7)	866(3)	585(9)
C7	3448(4)	9215(6)	1918(2)	500(8)
C8	2557(4)	8017(6)	2310(2)	483(7)
C9	2913(3)	6156(5)	2785(2)	418(7)
C10	4267(4)	5372(6)	2850(3)	531(9)
C11	4575(4)	3607(7)	3302(3)	533(8)
C12	3526(4)	2566(6)	3699(2)	459(7)
C13	2166(4)	3309(7)	3637(3)	542(8)
C14	1869(4)	5073(7)	3194(2)	527(8)
O1	3706(3)	807(5)	4156(2)	634(7)
C15	5043(6)	−122(9)	4170(4)	753(12)
O2	867(4)	3073(10)	8633(3)	1293(18)
O3	3261(5)	3300(10)	8503(3)	1367(18)
O4	2307(11)	515(8)	9191(3)	1904(32)
S	2121(.9)	1990	8564(.5)	489(2)
C16	1960(3)	626(5)	7597(2)	424(7)
C17	2128(4)	1657(6)	6845(2)	482(8)

I-1147-M22

Table S4A. (Cont.)

Atom	x	y	z	U_{eq}
C18	1955(4)	644(7)	6085(2)	565(9)
C19	1591(4)	−1435(7)	6056(2)	544(8)
C20	1450(4)	−2452(6)	6818(3)	554(9)
C21	1635(4)	−1443(6)	7583(3)	486(7)
C22	1376(6)	−2511(11)	5227(4)	828(14)

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

I-1147-M23

Table S4B. Assigned Parameters for 4'-Methoxy-N-methyl-4-stilbazolium Tosylate.

x, y and $z \times 10^4$

Atom	x	y	z	B
H2	4546(51)	15058(84)	460(29)	6.0
H3	5170(46)	11942(93)	1246(26)	5.5
H5	812(46)	10949(75)	1526(27)	5.2
H6	482(47)	14125(80)	752(26)	5.5
H7	4505(45)	8970(72)	1952(25)	4.7
H8	1512(43)	8514(70)	2313(25)	4.6
H10	5066(43)	6244(70)	2570(27)	5.0
H11	5542(48)	3196(73)	3342(26)	5.0
H13	1547(49)	2772(70)	3947(29)	5.1
H14	929(47)	5616(74)	3148(26)	5.0
H17	2365(45)	2995(73)	6863(26)	4.5
H18	2102(46)	1320(69)	5524(29)	5.2
H20	1109(48)	−3993(79)	6816(28)	5.2
H21	1643(44)	−2163(69)	8029(26)	4.6
H1A	1336(57)	17382(94)	367(32)	6.9
H1B	2001(53)	16186(81)	−515(35)	6.9
H1C	3127(56)	17516(94)	195(32)	6.9
H15A	5416(56)	−178(95)	3591(34)	7.1
H15B	4845(57)	−1401(95)	4501(32)	7.1
H15C	5868(58)	696(95)	4504(33)	7.1
H22A	530(58)	−2491(102)	5039(37)	7.8
H22B	1335(62)	−4105(106)	5325(39)	7.8
H22C	1995(64)	−2127(98)	4847(37)	7.8
O2A	1055	1372	9098	13.6
O3A	1964	4112	8407	13.6
O4A	3442	1554	8957	13.6

I-1147-m24

Table S4C. Anisotropic Displacement Parameters for 4'-Methoxy-N-methyl-4-stilbazolium Tosylate.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	1213(43)	472(25)	529(22)	60(24)	−62(25)	23(17)
N	781(23)	417(16)	457(15)	17(16)	15(15)	−30(13)
C2	749(28)	613(24)	533(20)	−105(22)	78(19)	41(18)
C3	583(21)	637(27)	543(19)	−15(20)	13(16)	35(18)
C4	545(20)	461(17)	411(16)	1(16)	−21(14)	−42(14)
C5	557(20)	518(21)	594(19)	11(19)	8(16)	17(18)
C6	662(23)	512(20)	579(21)	76(20)	−28(18)	−15(17)
C7	483(19)	475(18)	539(18)	20(15)	−53(15)	−6(15)
C8	442(17)	508(19)	496(18)	44(16)	−22(14)	−38(15)
C9	382(16)	429(16)	442(16)	−7(13)	−17(13)	−64(13)
C10	374(17)	560(21)	659(23)	−34(16)	−8(15)	48(18)
C11	345(16)	586(22)	666(22)	44(16)	−27(15)	61(18)
C12	507(17)	503(20)	363(16)	27(15)	−35(13)	−8(13)
C13	438(18)	623(23)	570(20)	4(17)	113(16)	113(18)
C14	394(18)	625(23)	562(20)	51(16)	37(15)	19(16)
O1	625(17)	645(17)	635(16)	64(14)	59(13)	181(14)
C15	718(29)	696(28)	838(31)	162(24)	−94(25)	169(25)
O2	624(24)	1910(62)	1339(41)	411(30)	−74(23)	−1031(42)
O3	965(34)	1829(60)	1341(42)	−907(38)	564(29)	−1042(42)
O4	4515(151)	611(26)	544(25)	231(51)	−576(46)	−8(19)
S	488(4)	472(4)	506(4)	−15(4)	16(3)	−70(4)
C16	351(15)	404(16)	516(18)	21(13)	0(13)	−19(14)
C17	425(17)	482(21)	541(18)	−25(15)	48(14)	46(15)
C18	488(19)	715(26)	494(20)	40(19)	34(16)	37(18)
C19	377(16)	692(24)	561(21)	51(17)	6(15)	−140(18)
C20	473(18)	403(20)	783(25)	33(15)	−18(17)	−120(16)
C21	526(18)	375(16)	556(20)	−4(16)	14(16)	36(15)
C22	634(25)	1111(48)	738(29)	−3(29)	−11(22)	−361(30)

The form of the displacement parameter is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

Table S4D. Complete Distances and Angles for
4'-Methoxy-N-methyl-4-stilbazolium Tosylate.

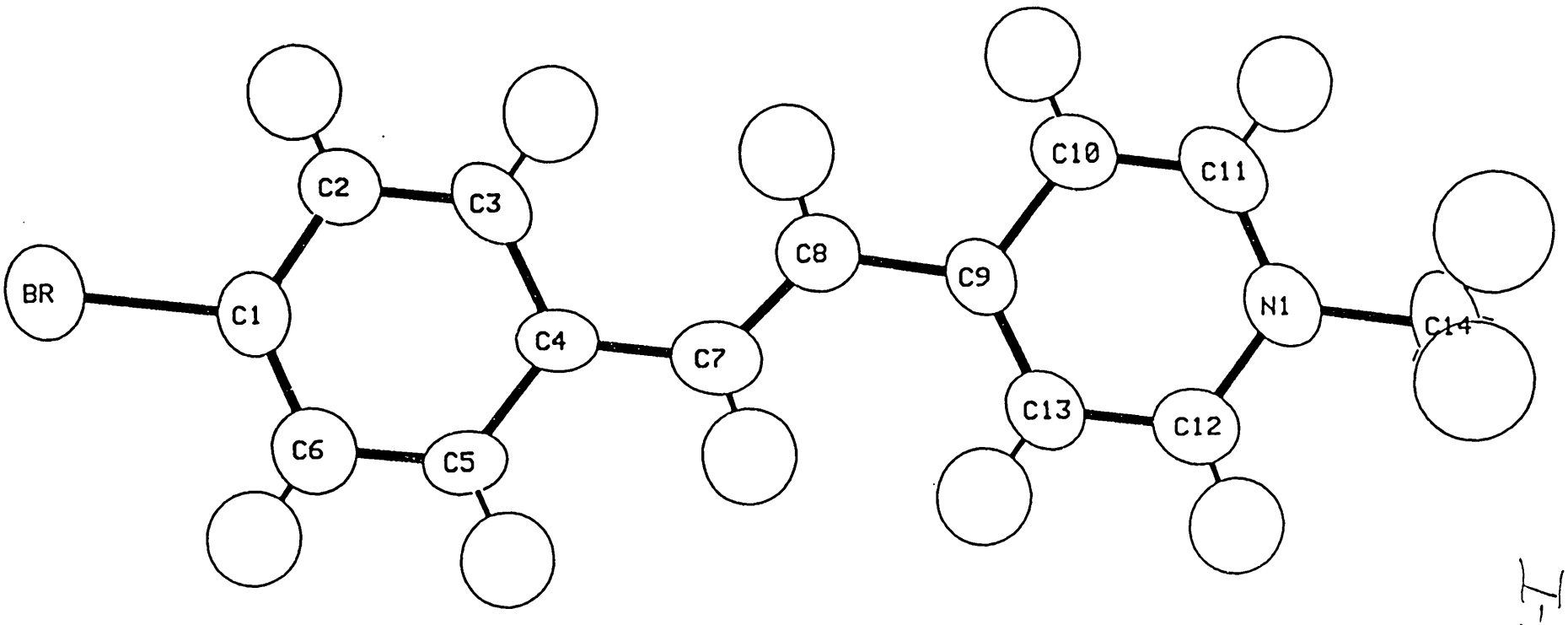
I-1147-m25

	Distance(Å)		Distance(Å)
C1 -N	1.481(6)	C19 -C20	1.391(6)
C1 -H1 A	1.07(6)	C19 -C22	1.501(7)
C1 -H1 B	1.01(5)	C20 -C21	1.389(6)
C1 -H1 C	1.10(6)	C20 -H20	1.06(5)
N -C2	1.346(6)	C21 -H21	0.85(4)
N -C6	1.347(5)	C22 -H22A	0.85(6)
C2 -C3	1.369(6)	C22 -H22B	1.05(6)
C2 -H2	1.02(5)	C22 -H22C	0.89(6)
C3 -C4	1.398(6)	C17 -H17	0.90(4)
C3 -H3	1.02(5)	C18 -C19	1.398(6)
C4 -C5	1.399(5)	C18 -H18	1.01(5)
C4 -C7	1.462(5)		
C5 -C6	1.371(6)		
C5 -H5	1.07(5)		
C6 -H6	1.01(5)		
C7 -C8	1.325(5)		
C7 -H7	1.02(4)		
C8 -C9	1.463(5)		
C8 -H8	1.05(4)		
C9 -C10	1.393(5)		
C9 -C14	1.399(5)		
C10 -C11	1.382(6)		
C10 -H10	1.06(4)		
C11 -C12	1.380(5)		
C11 -H11	0.96(5)		
C12 -C13	1.389(5)		
C12 -O1	1.364(5)		
C13 -C14	1.372(6)		
C13 -H13	0.86(5)		
C14 -H14	0.97(5)		
O1 -C15	1.414(6)		
C15 -H15A	1.00(6)		
C15 -H15B	1.01(6)		
C15 -H15C	1.08(6)		
O2 -S	1.398(5)		
O3 -S	1.391(6)		
O4 -S	1.392(7)		
S -C16	1.779(3)		
S -O2A	1.406		
S -O3A	1.411		
S -O4A	1.421		
C16 -C17	1.385(5)		
C16 -C21	1.382(5)		
C17 -C18	1.382(6)		

Table S4D. (Cont.)

I-1147-m26

	Angle(°)		Angle(°)
H1 A	-C1 -N	110.8(30)	
H1 B	-C1 -N	108.3(30)	
H1 C	-C1 -N	103.4(29)	
H1 B	-C1 -H1 A	113.7(42)	
H1 C	-C1 -H1 A	107.3(42)	
H1 C	-C1 -H1 B	112.9(42)	
C2	-N -C1	120.3(4)	
C6	-N -C1	118.9(4)	
C6	-N -C2	120.8(4)	
C3	-C2 -N	120.3(4)	
H2	-C2 -N	113.3(28)	
H2	-C2 -C3	126.3(28)	
C4	-C3 -C2	120.9(4)	
H3	-C3 -C2	117.8(28)	
H3	-C3 -C4	121.2(28)	
C5	-C4 -C3	116.8(3)	
C7	-C4 -C3	119.1(3)	
C7	-C4 -C5	124.1(3)	
C6	-C5 -C4	120.5(4)	
H5	-C5 -C4	122.7(24)	
H5	-C5 -C6	116.8(24)	
C5	-C6 -N	120.7(4)	
H6	-C6 -N	115.3(27)	
H6	-C6 -C5	124.1(27)	
C8	-C7 -C4	125.3(3)	
H7	-C7 -C4	112.3(25)	
H7	-C7 -C8	122.2(25)	
C9	-C8 -C7	126.0(3)	
H8	-C8 -C7	116.6(23)	
H8	-C8 -C9	117.3(23)	
C10	-C9 -C8	122.8(3)	
C14	-C9 -C8	120.0(3)	
C14	-C9 -C10	117.2(3)	
C11	-C10 -C9	121.7(4)	
H10	-C10 -C9	116.9(24)	
H10	-C10 -C11	121.2(24)	
C12	-C11 -C10	120.0(4)	
H11	-C11 -C10	117.1(27)	
H11	-C11 -C12	122.9(27)	
C13	-C12 -C11	119.3(3)	
O1	-C12 -C11	125.1(3)	
O1	-C12 -C13	115.7(3)	
C14	-C13 -C12	120.4(4)	
H13	-C13 -C12	118.6(31)	
H13	-C13 -C14	120.1(31)	
C13	-C14 -C9	121.4(4)	
H14	-C14 -C9	117.2(27)	
H14	-C14 -C13	121.4(27)	
C15	-O1 -C12	117.8(3)	
H15A	-C15 -O1	110.4(33)	
H15B	-C15 -O1	100.3(32)	
H15C	-C15 -O1	116.4(30)	
H15B	-C15 -H15A	122.1(46)	
H15C	-C15 -H15A	101.3(45)	
H15C	-C15 -H15B	107.3(44)	
O3	-S -O2	111.9(3)	
O4	-S -O2	112.5(4)	
C16	-S -O2	105.6(2)	
O4	-S -O3	112.9(4)	
C16	-S -O3	107.0(3)	
C16	-S -O4	106.3(3)	
O2A	-S -C16	109.6	
O3A	-S -C16	109.3	
O4A	-S -C16	109.4	
O3A	-S -O2A	108.2	
O4A	-S -O2A	109.2	
O4A	-S -O3A	111.2	
C17	-C16 -S	119.7(3)	
C21	-C16 -S	120.9(3)	
C21	-C16 -C17	119.4(3)	
C18	-C17 -C16	120.6(3)	
H17	-C17 -C16	118.5(28)	
H17	-C17 -C18	120.9(28)	
C19	-C18 -C17	121.0(4)	
H18	-C18 -C17	123.3(26)	
H18	-C18 -C19	115.7(26)	
C20	-C19 -C18	117.5(4)	
C22	-C19 -C18	120.6(4)	
C22	-C19 -C20	121.8(4)	
C21	-C20 -C19	121.6(4)	
H20	-C20 -C19	119.3(26)	
H20	-C20 -C21	118.8(26)	
C20	-C21 -C16	119.8(3)	
H21	-C21 -C16	121.8(29)	
H21	-C21 -C20	117.9(29)	
H22A	-C22 -C19	113.8(41)	
H22B	-C22 -C19	109.7(35)	
H22C	-C22 -C19	112.8(40)	
H22B	-C22 -H22A	91.6(53)	
H22C	-C22 -H22A	113.4(57)	
H22C	-C22 -H22B	113.9(53)	



Labelled drawing of the cation of 4′–bromo–N–methyl–4–stilbazolium chloride·$4H_2O$ with 50% probability ellipsoids.

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I-1147-M38

Table S5A. Final Heavy Atom Parameters for 4′-Bromo-N-methyl-4-stilbazolium Chloride.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq}
Br	3922(1)	2291(1)	0	737(3)
C1	4325(5)	2391(12)	1267(5)	495(23)
C2	3827(5)	2119(11)	2024(7)	550(26)
C3	4120(6)	2204(13)	2944(6)	564(27)
C4	4881(6)	2547(17)	3123(8)	454(26)
C5	5349(5)	2815(16)	2333(8)	511(32)
C6	5077(5)	2747(13)	1409(7)	602(28)
C7	5192(7)	2609(16)	4085(8)	544(34)
C8	4826(4)	2357(11)	4897(10)	524(20)
C9	5174(7)	2434(17)	5867(7)	458(31)
C10	4710(6)	2132(17)	6659(7)	570(32)
C11	5009(7)	2250(17)	7557(9)	665(33)
N1	5742(5)	2634(12)	7697(6)	526(21)
C12	6213(5)	2888(12)	6944(7)	586(27)
C13	5918(5)	2797(12)	6035(6)	544(25)
C14	6075(6)	2751(14)	8689(6)	839(32)
Cl	2456(1)	2261(3)	4383(2)	688(6)
O1	3054(7)	−576(17)	6022(8)	1042(36)
O2	2060(7)	−622(17)	2697(7)	1086(38)
O3	1935(7)	5534(13)	2943(8)	1085(38)
O4	3144(7)	5500(12)	5822(10)	909(30)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij} (a_i^* a_j^*) (\vec{a}_i \cdot \vec{a}_j)]$

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Table S5B. Hydrogen Atom Parameters for 4′-Bromo-N-methyl-4-stilbazolium Chloride.

x, y and $z \times 10^4$

Atom	x	y	z	B
HO1A	2937(90)	−1493(181)	5981(108)	12.2(64)
HO1B	3013(60)	104(128)	5600(63)	5.4(33)
HO2A	2009(57)	−1611(130)	2866(71)	5.2(34)
HO2B	2213(68)	53(162)	3129(83)	9.1(46)
HO3A	2021(54)	5280(111)	2416(56)	3.9(26)
HO3B	2117(62)	4673(146)	3218(76)	6.4(38)
HO4A	2887(76)	5119(186)	6230(100)	9.8(59)
HO4B	2755(54)	5151(131)	5492(60)	5.7(32)
H2	3308	1866	1900	6.0
H3	3770	2042	3467	6.0
H5	5875	3047	2436	6.0
H6	5413	2956	887	6.0
H7	5720	2825	4119	6.0
H8	4299	2092	4872	6.0
H10	4182	1865	6568	6.0
H11	4695	1966	8088	6.0
H12	6744	3128	7032	6.0
H13	6247	2994	5509	6.0
H14A	5691	2514	9145	10.0
H14B	6268	4001	8776	10.0
H14C	6469	1865	8743	10.0

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Table S5C. Anisotropic Displacement Parameters for 4′-Bromo-N-methyl-4-stilbazolium Chloride.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br	772(6)	914(7)	524(5)	52(8)	−10(9)	−11(21)
C1	594(62)	442(50)	449(55)	87(56)	−16(49)	−10(52)
C2	486(63)	607(61)	557(64)	76(59)	59(55)	−30(58)
C3	649(78)	584(59)	459(61)	67(64)	156(50)	11(53)
C4	368(63)	426(55)	569(73)	−5(59)	71(66)	58(70)
C5	304(66)	621(75)	608(74)	18(64)	56(71)	−27(65)
C6	615(75)	596(63)	595(71)	43(60)	44(50)	−24(62)
C7	521(87)	436(60)	674(103)	−1(75)	95(68)	−17(69)
C8	521(42)	472(47)	579(60)	12(46)	39(80)	0(85)
C9	518(91)	469(63)	386(73)	51(74)	61(64)	−19(71)
C10	553(79)	585(78)	571(79)	−83(62)	119(69)	−47(61)
C11	755(90)	694(81)	546(73)	−26(75)	206(73)	16(78)
N1	622(63)	501(47)	456(47)	80(53)	88(49)	15(50)
C12	534(69)	623(63)	601(66)	−11(57)	83(58)	20(60)
C13	597(69)	550(56)	485(56)	27(60)	70(53)	45(57)
C14	1042(79)	1093(79)	383(51)	44(94)	22(61)	12(61)
Cl	738(16)	776(15)	549(13)	5(20)	142(11)	5(26)
O1	1451(102)	774(73)	901(82)	−55(65)	−348(67)	158(60)
O2	1785(117)	733(69)	739(72)	111(70)	−154(68)	−45(58)
O3	1921(112)	673(64)	660(69)	50(61)	−276(71)	−16(54)
O4	1028(83)	848(59)	852(78)	−123(53)	−232(72)	−17(51)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table S5D. Complete Distances and Angles for 4'-Bromo-N-methyl-4-stilbazolium Chloride.

	Distance(Å)
BR -C1	1.906
C1 -C2	1.387(12)
C1 -C6	1.364(12)
C2 -C3	1.384(12)
C2 -H2	0.947
C3 -C4	1.387(14)
C3 -H3	0.961
C4 -C5	1.390(15)
C4 -C7	1.449(16)
C5 -C6	1.375(14)
C5 -H5	0.951
C6 -H6	0.951
C7 -C8	1.315(15)
C7 -H7	0.945
C8 -C9	1.486(14)
C8 -H8	0.950
C9 -C10	1.392(15)
C9 -C13	1.356(14)
C10 -C11	1.360(16)
C10 -H10	0.958
C11 -N1	1.336(14)
C11 -H11	0.947
N1 -C12	1.350(12)
N1 -C14	1.505(13)
C12 -C13	1.372(12)
C12 -H12	0.960
C13 -H13	0.947
C14 -H14A	0.944
C14 -H14B	0.955
C14 -H14C	0.938
O1 -HO1A	0.68(15)
O1 -HO1B	0.76(10)
O2 -HO2A	0.74(10)
O2 -HO2B	0.81(12)
O3 -HO3A	0.77(8)
O3 -HO3B	0.79(11)
O4 -HO4A	0.78(14)
O4 -HO4B	0.86(9)

	Angle(°)
C2 -C1 -BR	117.7(6)
C6 -C1 -BR	120.3(6)
C6 -C1 -C2	122.0(8)
C3 -C2 -C1	117.6(8)
H2 -C2 -C1	119.8(8)
H2 -C2 -C3	122.6(9)
C4 -C3 -C2	122.4(9)
H3 -C3 -C2	117.3(9)
H3 -C3 -C4	120.3(9)
C5 -C4 -C3	117.1(10)
C7 -C4 -C3	122.6(10)
C7 -C4 -C5	120.3(10)
C6 -C5 -C4	122.0(10)
H5 -C5 -C4	118.8(10)
H5 -C5 -C6	119.1(10)
C5 -C6 -C1	118.8(9)
H6 -C6 -C1	121.5(9)
H6 -C6 -C5	119.7(9)
C8 -C7 -C4	127.4(10)
H7 -C7 -C4	115.1(11)
H7 -C7 -C8	117.5(11)
C9 -C8 -C7	125.2(9)
H8 -C8 -C7	118.4(10)
H8 -C8 -C9	116.4(9)
C10 -C9 -C8	118.3(9)
C13 -C9 -C8	124.3(9)
C13 -C9 -C10	117.3(10)
C11 -C10 -C9	119.6(10)
H10 -C10 -C9	119.7(10)
H10 -C10 -C11	120.7(11)
N1 -C11 -C10	121.5(11)
H11 -C11 -C10	118.7(12)
H11 -C11 -N1	119.7(11)
C12 -N1 -C11	120.5(9)
C14 -N1 -C11	121.6(9)
C14 -N1 -C12	117.9(8)
C13 -C12 -N1	118.6(8)
H12 -C12 -N1	121.6(9)
H12 -C12 -C13	119.8(9)
C12 -C13 -C9	122.4(9)
H13 -C13 -C9	119.1(9)
H13 -C13 -C12	118.5(8)
H14A -C14 -N1	109.2(8)
H14B -C14 -N1	107.8(8)
H14C -C14 -N1	109.0(8)
H14B -C14 -H14A	109.6(9)
H14C -C14 -H14A	111.1(10)

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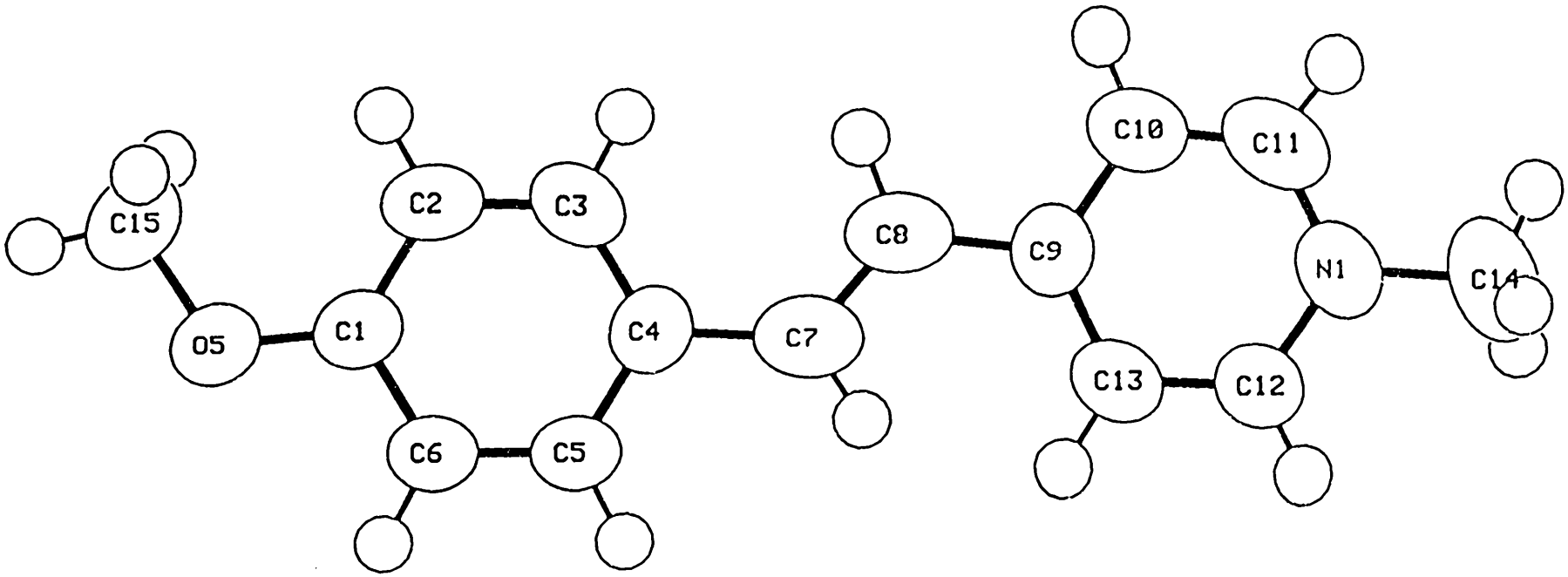
Table S5D. (Cont.)

			Angle(°)
H14C	-C14	-H14B	110.1(10)
HO1B	-O1	-HO1A	120.3(142)
HO2B	-O2	-HO2A	110.9(112)
HO3B	-O3	-HO3A	101.7(100)
HO4B	-O4	-HO4A	80.0(117)



Labelled drawing of the cation of 4′–methoxy–N–methyl–4–stilbazolium chloride·4H_2O with 50% probability ellipsoids. Hydrodgen atoms are shown with arbitrary, small thermal parameters.

I-1147-m33

I-1147-m34

Table S6A. Final Heavy Atom Parameters for 4'-Methoxy-N-methyl-4-stilbazolium Chloride.

	x, y, z and U_{eq}[a] $\times 10^4$			
Atom	x	y	z	U_{eq}
Cl	2433(1)	2167(1)	4366	750(2)
C15	3641(3)	2104(7)	13(4)	967(14)
O5	4374(2)	2459(4)	319(3)	764(8)
C1	4511(2)	2460(5)	1273(3)	593(11)
C2	3994(2)	2106(5)	1992(4)	676(12)
C3	4221(2)	2170(5)	2938(4)	684(12)
C4	4948(2)	2551(5)	3189(3)	614(11)
C5	5443(2)	2889(6)	2469(3)	654(12)
C6	5233(2)	2851(6)	1533(3)	655(12)
C7	5217(2)	2600(6)	4203(4)	763(13)
C8	4841(3)	2289(6)	4983(4)	783(13)
C9	5152(3)	2382(5)	5949(3)	644(11)
C10	4697(3)	2036(6)	6724(4)	768(14)
C11	4966(3)	2182(6)	7607(4)	839(16)
N1	5662(2)	2649(5)	7790(3)	725(10)
C12	6119(2)	2965(6)	7054(4)	710(12)
C13	5886(2)	2845(5)	6132(4)	682(12)
C14	5941(3)	2769(7)	8777(4)	1045(18)
O1	3087(3)	−572(7)	5974(3)	1081(14)
O2	2197(3)	−665(7)	2630(3)	1269(15)
O3	2103(3)	5503(6)	2838(4)	1297(19)
O4	3087(2)	5448(5)	5770(3)	948(10)

[a] $U_{eq} = \frac{1}{3} \sum_i \sum_j [U_{ij} (a_i^* a_j^*) (\vec{a}_i \cdot \vec{a}_j)]$

Table S6B. Hydrogen Atom Parameters for 4′-Methoxy-N-methyl-4-stilbazolium Chloride.

x, y and $z \times 10^4$

Atom	x	y	z	B
HO1A	3120(24)	−1476(54)	5861(35)	4.7(12)
HO1B	2885(36)	67(95)	5652(45)	11.4(23)
HO2A	2092(34)	−2083(10)	2782(46)	13.5(22)
HO2B	2277(24)	103(79)	3159(37)	8.7(13)
HO3A	2012(29)	5230(81)	2329(41)	8.7(17)
HO3B	2225(23)	4854(65)	3125(31)	5.3(12)
HO4A	2836(37)	4739(10)	6529(55)	16.9(24)
HO4B	2895(35)	4701(95)	5424(50)	12.2(22)
H2	3497	1848	1835	5.6
H3	3860	1970	3411	5.6
H5	5941	3149	2629	5.6
H6	5595	3110	1051	5.6
H7	5701	2902	4399	6.4
H8	4328	1963	4908	6.4
H10	4190	1686	6655	6.6
H11	4671	1932	8139	6.6
H12	6617	3271	7180	6.6
H13	6234	3111	5623	6.6
H14A	6242	3853	8822	8.9
H14B	6226	1641	8894	8.9
H14C	5542	2826	9208	8.9
H15A	3312	2847	356	8.5
H15B	3535	761	113	8.5
H15C	3599	2340	−665	8.5

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Table S6C. Anisotropic Displacement Parameters for 4′-Methoxy-N-methyl-4-stilbazolium Chloride.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl	889(7)	756(5)	604(5)	15(6)	49(5)	−14(9)
C15	753(29)	1182(38)	966(36)	−8(26)	−172(28)	−29(29)
O5	613(17)	883(19)	797(23)	9(14)	−41(15)	−13(14)
C1	566(24)	426(23)	786(30)	46(18)	−17(24)	7(18)
C2	510(26)	533(24)	984(39)	32(18)	94(25)	24(21)
C3	741(31)	561(24)	750(33)	55(20)	212(24)	54(21)
C4	708(29)	430(21)	703(28)	12(19)	−72(24)	−34(19)
C5	537(26)	637(28)	788(31)	−52(18)	53(25)	5(21)
C6	561(26)	640(27)	764(33)	−39(18)	74(21)	−7(22)
C7	708(27)	468(23)	1112(40)	14(18)	157(29)	−32(24)
C8	647(24)	620(29)	1081(43)	1(18)	149(28)	−43(27)
C9	802(30)	466(22)	663(29)	52(21)	−39(25)	−34(20)
C10	752(31)	648(30)	905(38)	35(21)	152(30)	40(24)
C11	974(42)	625(29)	917(44)	68(26)	340(33)	52(24)
N1	966(29)	572(20)	637(24)	67(18)	100(24)	−9(17)
C12	740(27)	675(28)	714(31)	−20(20)	71(26)	41(21)
C13	752(31)	564(25)	729(33)	4(21)	156(23)	30(22)
C14	1561(55)	877(37)	697(35)	139(30)	71(34)	5(25)
O1	1482(37)	759(29)	1001(30)	100(26)	−454(25)	−44(26)
O2	2240(41)	823(28)	744(25)	126(28)	−163(24)	−118(19)
O3	2392(60)	648(28)	852(35)	−116(27)	−252(33)	84(22)
O4	1062(24)	792(22)	990(25)	−181(18)	−266(20)	11(19)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table S6D. Complete Distances and Angles for 4'-Methoxy-N-methyl-4-stilbazolium Chloride.

Distance(Å)		Angle(°)	
C15 –O5	1.420(6)	H15A –C15 –O5	110.6(4)
C15 –H15A	0.927	H15B –C15 –O5	108.3(4)
C15 –H15B	0.975	H15C –C15 –O5	109.8(4)
C15 –H15C	0.965	H15B –C15 –H15A	110.1(5)
O5 –C1	1.355(5)	H15C –C15 –H15A	111.0(5)
C1 –C2	1.397(6)	H15C –C15 –H15B	107.0(5)
C1 –C6	1.387(6)	C1 –O5 –C15	117.9(3)
C2 –C3	1.385(6)	C2 –C1 –O5	125.6(4)
C2 –H2	0.946	C6 –C1 –O5	115.5(3)
C3 –C4	1.391(6)	C6 –C1 –C2	118.9(4)
C3 –H3	0.941	C3 –C2 –C1	118.6(4)
C4 –C5	1.368(6)	H2 –C2 –C1	120.7(4)
C4 –C7	1.498(6)	H2 –C2 –C3	120.7(4)
C5 –C6	1.361(6)	C4 –C3 –C2	121.9(4)
C5 –H5	0.950	H3 –C3 –C2	117.1(4)
C6 –H6	0.959	H3 –C3 –C4	120.9(4)
C7 –C8	1.304(7)	C5 –C4 –C3	118.2(4)
C7 –H7	0.946	C7 –C4 –C3	123.4(4)
C8 –C9	1.463(6)	C7 –C4 –C5	118.4(4)
C8 –H8	0.966	C6 –C5 –C4	121.1(4)
C9 –C10	1.383(6)	H5 –C5 –C4	119.1(4)
C9 –C13	1.396(6)	H5 –C5 –C6	119.8(4)
C10 –C11	1.329(7)	C5 –C6 –C1	121.3(4)
C10 –H10	0.957	H6 –C6 –C1	120.2(4)
C11 –N1	1.331(6)	H6 –C6 –C5	118.5(4)
C11 –H11	0.932	C8 –C7 –C4	128.0(4)
N1 –C12	1.339(6)	H7 –C7 –C4	125.6(4)
N1 –C14	1.471(7)	H7 –C7 –C8	106.3(4)
C12 –C13	1.358(6)	C9 –C8 –C7	124.1(4)
C12 –H12	0.946	H8 –C8 –C7	116.9(5)
C13 –H13	0.969	H8 –C8 –C9	118.9(4)
C14 –H14A	0.940	C10 –C9 –C8	118.8(4)
C14 –H14B	0.961	C13 –C9 –C8	123.2(4)
C14 –H14C	0.944	C13 –C9 –C10	118.0(4)
O1 –HO1A	0.66(4)	C11 –C10 –C9	119.4(4)
O1 –HO1B	0.73(7)	H10 –C10 –C9	122.7(5)
O2 –HO2A	1.04(7)	H10 –C10 –C11	117.9(5)
O2 –HO2B	0.93(5)	N1 –C11 –C10	123.1(5)
O3 –HO3A	0.75(6)	H11 –C11 –C10	120.8(5)
O3 –HO3B	0.65(4)	H11 –C11 –N1	116.1(5)
O4 –HO4A	1.26(7)	C12 –N1 –C11	118.9(4)
O4 –HO4B	0.79(7)	C14 –N1 –C11	121.5(4)
		C14 –N1 –C12	119.6(4)
		C13 –C12 –N1	121.6(4)
		H12 –C12 –N1	119.2(4)
		H12 –C12 –C13	119.2(4)
		C12 –C13 –C9	119.0(4)

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Table S6D. (Cont.)

Angle(°)

H13	-C13	-C9	122.3(4)
H13	-C13	-C12	118.7(4)
H14A	-C14	-N1	108.0(5)
H14B	-C14	-N1	107.3(5)
H14C	-C14	-N1	109.5(5)
H14B	-C14	-H14A	110.2(5)
H14C	-C14	-H14A	111.8(5)
H14C	-C14	-H14B	109.8(5)
HO1B	-O1	-HO1A	119.4(63)
HO2B	-O2	-HO2A	115.2(48)
HO4A	-O2	-HO2A	111.7(45)
HO4A	-O2	-HO2B	133.1(41)
HO3B	-O3	-HO3A	118.6(58)
HO4B	-O4	-HO4A	95.2(58)

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Table S2E. Observed and Calculated Structure Factors for 4′-Dimethylamino-N-methyl-4-stilbazolium Tosylate

The columns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

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-12 0 1

2	46	46	0
4	35	41	-5

-12 2 1

1	44	40	4
2	45	48	-4
3	41	46	-7
4	68	57	18

-11 1 1

1	117	116	3
2	55	49	9
3	29	34	-6
4	-9	35	-26
5	53	61	-13
6	43	50	-10
7	89	95	-14
8	40	43	-3
9	66	59	13
10	-7	20	-8

-11 3 1

1	62	52	17
2	34	37	-4
3	45	50	-7
4	86	77	18
5	48	46	3
6	111	104	16
7	13	17	-1
8	90	80	19
9	43	33	11

-11 5 1

1	-19	16	-12
2	122	114	19
3	27	11	10
4	99	88	23
5	27	28	0
6	67	64	4

-10 0 1

2	129	115	26
4	94	103	-15
6	133	126	12
8	60	51	11
10	90	84	9
12	99	97	2

-10 2 1

1	77	87	-24
2	60	59	1
3	125	122	7
4	12	13	0
5	-12	29	-21
6	121	119	4
7	141	147	-18
8	45	50	-7
9	77	67	19
10	58	58	1
11	92	92	0
12	95	87	15

-10 4 1

1	89	102	-31
2	99	93	14
3	198	185	33
4	54	49	9
5	51	43	13
6	51	45	9
7	159	159	1
8	41	27	16
9	106	97	20
10	20	30	-6
11	77	75	5

-10 6 1

1	127	111	37
2	88	84	9
3	87	90	-6
4	126	122	9
5	207	203	9
6	186	176	25
7	42	53	-16
8	87	94	-14

-9 1 1

1	22	31	-10
2	40	43	-5
3	82	79	7
4	92	90	6
5	177	180	-9
6	28	27	0
7	88	86	6
8	99	107	-21
9	105	110	-13
10	52	56	-7
11	31	42	-14
12	29	39	-12
13	47	44	4
14	31	37	-7
15	-30	25	-28

-9 3 1

1	133	139	-17
2	178	184	-15
3	247	248	-1
4	256	244	30
5	187	180	18
6	236	234	3
7	210	203	19
8	307	306	2
9	124	127	-9
10	95	98	-3
11	74	73	2
12	72	62	17
13	-17	10	-7
14	97	91	11

-9 5 1

1	54	54	0
2	89	82	17
3	78	73	11
4	113	112	2
5	0	19	-7
6	165	164	2
7	88	83	10
8	127	115	29
9	34	32	2
10	132	127	9
11	27	21	5
12	84	92	-17

-9 7 1

1	8	10	0
2	36	33	3
3	109	107	4
4	42	40	3
5	31	31	0
6	67	70	-5
7	44	56	-20
8	-31	8	-20
9	83	82	1
10	25	43	-14

-9 9 1

1	18	42	-25
2	-17	4	-5
3	47	49	-1

-8 0 1

2	131	126	11
4	691	673	23
6	564	557	10
8	692	699	-8
10	249	255	-11
12	164	166	-3
14	155	149	11
16	83	72	15

-8 2 1

1	167	166	5
2	63	64	-4
3	46	42	6
4	33	41	-12
5	195	203	-23
6	199	197	7
7	126	130	-13
8	10	14	-1
9	181	175	16
10	133	128	13
11	143	143	0
12	96	88	20
13	114	97	38
14	55	56	-1
15	-23	13	-13
16	75	80	-10

-8 4 1

1	47	52	-8
2	109	113	-11
3	53	45	16
4	80	83	-7
5	130	134	-11
6	139	130	25
7	27	31	-5
8	136	132	11
9	173	171	6
10	51	60	-16
11	26	25	0
12	79	79	0
13	99	92	15
14	55	58	-5
15	82	67	27

-8 6 1

1	214	218	-11
2	95	99	-11
3	83	92	-22
4	114	104	25
5	58	58	0
6	-6	11	-3
7	54	49	9
8	97	93	8
9	110	102	20
10	58	58	0
11	125	118	17
12	70	72	-3
13	109	100	20

-8 8 1

1	68	65	6
2	107	103	8
3	51	48	3
4	54	51	4
5	27	39	-14
6	55	51	6
7	41	34	7
8	96	90	12
9	-23	31	-29
10	57	54	5

-8 10 1

1	51	57	-10
2	73	85	-23
3	23	22	1
4	48	56	-8

-7 1 1

1	166	157	28
2	118	117	2
3	188	179	27
4	51	52	-3
5	224	226	-6
6	161	161	0
7	39	44	-10
8	189	195	-17
9	221	223	-6
10	24	30	-7
11	56	56	0
12	132	139	-19
13	90	92	-4
14	110	105	13
15	112	107	11
16	56	57	-1
17	95	95	0

-7 3 1

1	156	169	-43
2	337	329	18
3	304	305	-1
4	57	51	14
5	166	168	-6
6	672	677	-7
7	420	422	-4
8	115	115	0
9	238	240	-4
10	459	460	-2
11	180	186	-16
12	107	103	10
13	65	62	5
14	182	188	-16
15	127	126	1
16	76	77	-2
17	29	18	8

-7 5 1

1	125	119	18
2	313	305	19
3	128	121	20
4	381	389	-18
5	137	128	23
6	241	242	-2
7	61	49	24
8	212	216	-9
9	44	34	15
10	198	203	-13
11	-6	28	-17
12	101	101	1
13	122	117	13
14	112	118	-15
15	-26	10	-16
16	89	87	5

-7 7 1

1	32	18	14
2	204	197	18

3	42	42	0
4	122	127	-14
5	-6	17	-7
6	66	74	-17
7	56	62	-11
8	106	113	-18
9	109	111	-4
10	77	71	12
11	25	26	-1
12	22	37	-15
13	17	33	-14
14	82	82	0

-7 9 1

1	143	130	31
2	135	134	1
3	68	70	-4
4	57	52	8
5	115	115	0
6	46	55	-15
7	56	62	-10
8	-22	19	-18
9	56	60	-7
10	16	36	-17

-7 11 1

1	37	41	-4
2	108	95	23

-6 0 1

2	211	200	28
4	193	189	10
6	133	135	-4
8	153	158	-12
10	78	91	-27
12	244	250	-13
14	248	264	-32
16	201	212	-21
18	152	157	-9

-6 2 1

1	426	419	14
2	110	102	25
3	163	164	-4
4	220	221	-2
5	131	129	7
6	225	225	0
7	188	196	-25
8	223	221	7
9	89	94	-12
10	151	159	-26
11	166	153	37
12	149	145	10
13	88	78	23
14	157	162	-12
15	215	219	-11
16	102	84	38
17	141	136	10
18	109	110	-1

-6 4 1

1	200	203	-9
2	12	11	0
3	333	333	3
4	88	85	8
5	364	368	-11
6	160	161	-3
7	272	273	0
8	110	104	17
9	374	370	10
10	254	253	2
11	282	278	8
12	60	61	0
13	208	209	-1
14	92	86	13
15	282	278	9
16	86	82	7
17	142	142	0

-6 6 1

1	178	180	-6
2	112	116	-12
3	243	233	26
4	183	175	22
5	205	205	0
6	316	315	2
7	519	518	2
8	350	350	0
9	167	166	1
10	266	256	24
11	364	370	-13
12	59	58	2
13	152	145	17
14	50	46	7
15	157	162	-13
16	27	30	-3

-6 8 1

1	-16	25	-21
2	84	78	12
3	69	77	-20
4	194	194	0
5	128	123	13
6	77	78	-1
7	52	48	5
8	153	160	-17
9	42	38	5
10	101	102	-1
11	40	54	-23
12	44	62	-32
13	9	36	-21

-6 10 1

1	38	30	10
2	80	79	1
3	93	97	-9
4	23	31	-7
5	19	36	-18
6	83	84	-1
7	119	132	-31
8	72	67	10
9	50	38	16
10	36	13	17

-5 1 1

1	759	735	35
2	587	572	27
3	666	657	15
4	173	174	-2
5	463	460	5
6	196	194	6
7	403	402	2
8	152	158	-22
9	260	258	5
10	181	181	2
11	220	219	2
12	68	72	-9
13	209	212	-10
14	112	119	-19
15	202	213	-29
16	-26	24	-28
17	119	120	-1
18	45	67	-41
19	101	109	-19

-5 3 1

1	98	85	44
2	450	447	7
3	176	175	3
4	277	276	0
5	175	175	-1
6	249	247	3
7	227	227	-1
8	284	282	4
9	191	191	-2
10	185	191	-17
11	70	80	-25
12	182	185	-9
13	169	184	-43
14	127	119	19
15	57	72	-32
16	217	221	-12
17	94	106	-29
18	32	26	5
19	71	61	17

-5 5 1

1	317	316	2
2	223	215	26
3	20	26	-7
4	270	272	-5
5	167	166	0
6	147	156	-32
7	53	56	-6
8	438	434	8
9	23	22	1
10	127	126	2
11	67	73	-15
12	165	164	2
13	72	80	-18
14	170	158	30
15	90	86	9
16	116	114	5
17	22	32	-9
18	110	108	4

-5 7 1

1	149	144	14
2	81	82	0
3	164	166	-5
4	163	162	2
5	99	97	6
6	244	246	-5
7	333	338	-6
8	125	125	0
9	75	69	13
10	95	95	1
11	241	248	-18
12	135	134	3
13	120	119	0
14	55	47	12
15	84	87	-5
16	23	23	0

-5 9 1

1	108	108	0
2	72	72	1
3	144	135	23
4	31	30	0
5	238	240	-7
6	187	181	13
7	120	110	25
8	188	185	10
9	346	342	9
10	192	184	19
11	107	105	6
12	40	47	-10
13	147	152	-11

-5 11 1

1	117	124	-17
2	38	35	2
3	100	95	12
4	39	48	-14
5	27	33	-6
6	60	45	23
7	71	81	-19
8	72	69	6
9	83	83	0

-4 0 1

2	932	925	6
4	626	608	26
6	452	463	-20
8	329	310	41
10	329	336	-14
12	315	317	-5
14	418	417	3
16	322	319	5
18	207	213	-10
20	223	220	5

-4 2 1

1	726	719	11
2	539	525	28
3	396	390	13
4	311	304	21
5	73	77	-12
6	331	338	-20
7	374	371	8
8	363	371	-19
9	111	119	-28
10	282	282	0
11	135	142	-21
12	228	225	8
13	259	256	7
14	229	238	-26
15	146	141	14
16	157	152	13
17	188	190	-4
18	158	159	-1
19	109	109	0
20	80	88	-17

-4 4 1

1	262	265	-10
2	501	506	-9
3	183	178	17
4	255	246	29
5	359	354	10
6	311	304	19
7	76	78	-4
8	377	375	5
9	332	321	29
10	177	181	-12
11	146	153	-22
12	48	59	-25
13	234	232	6
14	78	87	-22
15	87	80	17
16	69	70	-2
17	197	202	-11
18	-8	35	-25
19	95	88	14

-4 6 1

1	136	133	11
2	323	324	-2
3	87	89	-5
4	34	26	12
5	176	170	18
6	179	178	2
7	213	212	2
8	112	111	5

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9	209	209	0
10	105	108	-6
11	187	190	-8
12	34	42	-12
13	102	101	4
14	162	169	-18
15	124	127	-5
16	80	86	-14
17	60	62	-3

-4 8 1

1	102	109	-21
2	123	123	0
3	90	93	-7
4	201	199	8
5	-23	5	-14
6	217	219	-8
7	99	99	-1
8	214	205	24
9	145	134	27
10	255	253	4
11	60	53	12
12	45	41	5
13	125	127	-3
14	159	159	0
15	14	15	0

-4 10 1

1	89	86	7
2	107	109	-4
3	81	81	0
4	146	145	3
5	62	65	-5
6	126	125	2
7	92	89	5
8	173	182	-23
9	60	54	10
10	123	120	7
11	73	71	3
12	252	245	16

-4 12 1

1	10	7	0
2	58	63	-8
3	67	78	-20
4	-19	24	-18
5	71	75	-7
6	96	108	-29

-3 1 1

1	970	960	12
2	194	181	50
3	697	692	8
4	389	385	11
5	428	445	-42
6	568	552	29
7	127	130	-8
8	765	743	31
9	277	274	8
10	222	221	3
11	150	151	-4
12	56	57	-1
13	245	243	6
14	63	67	-9
15	268	263	13
16	139	140	-2
17	181	182	-4
18	77	86	-20
19	41	65	-42
20	24	36	-12

-3 3 1

1	90	82	30
2	146	151	-18
3	98	102	-13
4	363	369	-16
5	232	240	-25
6	13	50	-68
7	304	309	-14
8	301	290	31
9	118	124	-20
10	101	101	-1
11	236	239	-9
12	207	208	-4
13	55	67	-27
14	104	106	-5
15	20	26	-6
16	182	179	7
17	47	54	-11
18	100	107	-16
19	89	82	14
20	89	81	15

-3 5 1

1	251	260	-29
2	472	455	36
3	388	387	4
4	118	119	-2
5	43	40	7
6	279	286	-21
7	85	81	12
8	50	65	-38
9	106	106	-2
10	171	166	17
11	47	60	-30
12	197	194	10
13	123	120	6
14	115	125	-30
15	119	121	-5
16	116	110	14
17	38	25	13
18	64	60	7
19	-20	25	-19

-3 7 1

1	313	316	-8
2	244	244	-2
3	95	104	-28
4	60	60	-1
5	212	214	-5
6	77	84	-22
7	228	227	3
8	105	110	-14
9	116	122	-18
10	195	193	5
11	288	281	16
12	178	178	-1
13	219	218	1
14	227	221	16
15	251	244	16
16	93	99	-15
17	130	135	-11

-3 9 1

1	148	151	-10
2	181	173	21
3	168	173	-14
4	74	72	5
5	211	201	26
6	38	33	5
7	174	172	7
8	40	48	-14
9	135	131	9
10	23	17	4
11	160	155	11
12	23	27	-3
13	71	65	11
14	39	47	-10
15	115	115	0

-3 11 1

1	143	138	14
2	50	47	4
3	-29	10	-21
4	85	75	21
5	37	35	2
6	66	74	-17
7	87	87	1
8	62	59	5
9	-24	5	-12
10	135	137	-5
11	-27	8	-14

-3 13 1

1	39	39	0
2	41	50	-9

-2 0 1

2	1055	1034	20
4	962	982	-20
6	343	326	39
8	250	252	-7
10	192	212	-52
12	291	289	4
14	273	277	-8
16	360	361	-2
18	127	115	22
20	68	80	-18

-2 2 1

1	512	501	23
2	681	694	-21
3	462	467	-10
4	609	629	-36
5	377	380	-7
6	234	239	-18
7	385	378	20
8	668	656	19
9	409	404	11
10	125	119	19
11	312	301	29
12	348	347	1
13	265	260	12
14	77	75	3
15	103	119	-45
16	163	167	-9
17	182	177	12
18	22	14	5
19	100	101	-2
20	96	90	12

-2 4 1

1	445	451	-13
2	289	291	-7
3	519	519	0
4	236	239	-11
5	530	541	-23
6	417	405	26
7	303	301	5
8	69	62	16
9	487	475	25
10	153	152	3
11	231	235	-11
12	312	307	13
13	423	416	14
14	182	190	-22
15	351	347	7
16	302	308	-14
17	198	199	-2
18	35	44	-13
19	88	92	-8
20	19	25	-3

-2 6 1

1	681	674	11
2	528	538	-20
3	218	214	13
4	138	137	4
5	299	304	-12
6	72	77	-16
7	293	298	-13
8	207	212	-16
9	304	299	12
10	103	97	15
11	71	76	-12
12	109	116	-20
13	126	122	11
14	150	149	0
15	139	135	10
16	-17	26	-21
17	53	45	11
18	84	81	5

-2 8 1

1	214	217	-10
2	150	144	17
3	152	143	27
4	179	172	21
5	95	96	-3
6	244	244	1
7	66	70	-9
8	200	202	-6
9	-20	10	-12
10	145	145	1
11	74	69	11
12	164	166	-5
13	88	95	-16
14	42	54	-18
15	62	78	-32
16	79	75	9

-2 10 1

1	50	54	-6
2	178	177	2
3	133	138	-14
4	-31	3	-23
5	49	54	-8
6	130	138	-22
7	50	44	9
8	76	76	0
9	89	87	6
10	84	82	4
11	-21	34	-32
12	40	47	-9
13	-1	21	-7

-2 12 1

1	62	52	16
2	44	49	-9
3	99	106	-16
4	51	59	-13
5	151	142	22
6	69	62	11
7	56	62	-11
8	-19	24	-18
9	62	62	0

-1 1 1

1	845	853	-10
2	677	677	0
3	555	551	7
4	167	148	83
5	156	147	40
6	596	581	26

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7	187	183	12
8	116	115	3
9	124	130	-25
10	19	14	6
11	44	34	19
12	310	317	-19
13	483	479	7
14	520	522	-3
15	115	118	-9
16	318	311	17
17	364	354	20
18	185	185	0
19	62	57	9
20	52	60	-14
21	60	52	13

-1 3 1

1	1303	1318	-13
2	1416	1421	-4
3	283	283	-1
4	118	102	64
5	355	360	-13
6	300	313	-42
7	590	599	-17
8	128	145	-69
9	424	422	5
10	168	165	9
11	209	218	-29
12	175	179	-13
13	147	136	33
14	284	282	2
15	187	183	10
16	239	231	20
17	20	39	-23
18	105	98	16
19	140	138	3
20	76	81	-9

-1 5 1

1	492	493	-2
2	166	152	50
3	192	196	-14
4	309	309	1
5	304	305	-1
6	435	434	0
7	219	215	13
8	515	513	5
9	367	358	21
10	355	358	-8
11	78	79	-1
12	434	437	-5
13	178	184	-17
14	154	158	-11
15	78	84	-14
16	173	171	3
17	81	88	-15
18	185	172	31
19	34	29	4

-1 7 1

1	233	243	-32
2	52	53	-2
3	249	251	-4
4	123	120	8
5	298	288	26
6	212	207	17
7	334	331	7
8	122	115	20
9	305	300	11
10	135	140	-12
11	147	145	7
12	37	33	5
13	179	177	5
14	37	43	-9
15	44	51	-10
16	-12	23	-13
17	83	87	-7
18	50	49	1

-1 9 1

1	134	136	-6
2	126	125	1
3	316	320	-10
4	221	218	10
5	10	19	-6
6	67	68	-1
7	313	316	-5
8	211	212	-2
9	100	92	21
10	50	51	-1
11	93	90	8
12	57	76	-41
13	73	71	3
14	28	45	-21
15	14	22	-5

-1 11 1

1	65	77	-27
2	160	157	7
3	118	116	6
4	16	36	-21
5	73	71	4
6	159	162	-6
7	-8	25	-14
8	52	42	14
9	50	51	-1
10	53	64	-21
11	26	30	-3
12	29	40	-13

-1 13 1

1	70	82	-25
2	20	18	1
3	46	47	-2
4	76	76	0
5	47	49	-3

0 0 1

2	487	517	-62
4	2886	3147	-95
6	1497	1541	-29
8	699	708	-13
10	625	634	-12
12	819	819	0
14	392	392	0
16	401	392	16
18	297	306	-16
20	83	98	-15

0 2 1

0	873	894	-28
1	747	751	-5
2	1540	1545	-3
3	923	943	-25
4	1051	1068	-19
5	339	347	-24
6	638	649	-20
7	257	243	45
8	638	646	-17
9	223	229	-22
10	448	447	2
11	370	373	-6
12	298	291	21
13	292	297	-13
14	404	404	0
15	556	563	-12
16	241	244	-8
17	273	270	5
18	239	238	3
19	122	123	-2
20	117	113	10
21	75	70	8

0 4 1

0	716	700	25
1	404	396	20
2	238	249	-43
3	174	172	6
4	127	139	-50
5	140	146	-20
6	204	207	-13
7	71	85	-49
8	241	239	5
9	126	112	43
10	184	174	30
11	189	193	-12
12	85	94	-28
13	121	120	0
14	146	151	-13
15	172	170	7
16	62	60	3
17	47	48	-1
18	23	24	-1
19	165	155	25
20	49	35	18

0 6 1

0	417	422	-11
1	37	28	16
2	138	146	-31
3	236	232	10
4	356	349	17
5	432	434	-3
6	215	206	27
7	524	525	0
8	278	273	16
9	179	180	-3
10	177	175	7
11	159	159	-2
12	226	230	-12
13	82	79	6
14	140	144	-10
15	40	35	5
16	98	101	-7
17	42	48	-8
18	124	117	18
19	81	83	-4

0 8 1

0	309	311	-6
1	225	227	-4
2	196	201	-13
3	236	236	1
4	328	322	16
5	166	170	-14
6	465	476	-21
7	327	325	4
8	177	178	-5
9	36	31	5
10	433	429	8
11	229	221	19
12	113	114	-2
13	114	112	5
14	148	151	-8
15	67	60	11
16	126	121	13
17	70	74	-8

0 10 1

0	279	279	0
1	120	120	0
2	267	273	-15
3	129	122	17
4	323	316	17
5	36	28	11
6	187	189	-5
7	82	83	-2
8	293	294	-2
9	65	63	3
10	128	128	-1
11	32	42	-14
12	163	158	10
13	66	68	-2
14	128	123	12

0 12 1

0	48	52	-5
1	45	48	-5
2	90	96	-15
3	41	45	-5
4	38	53	-24
5	56	49	12
6	24	34	-10
7	68	74	-12
8	-25	37	-39
9	-25	6	-12

1 1 1

0	264	260	17
1	1035	1022	14
2	484	477	16
3	1159	1163	-4
4	215	206	35
5	1018	1028	-11
6	303	294	26
7	446	443	6
8	247	259	-40
9	754	767	-19
10	133	131	10
11	656	660	-6
12	120	121	-2
13	415	417	-6
14	337	337	0
15	637	638	-1
16	157	152	14
17	252	251	2
18	132	137	-11
19	284	284	-1
20	115	103	26
21	180	178	2

1 3 1

0	1711	1735	-17
1	1375	1377	-1
2	1621	1644	-16
3	1123	1125	-2
4	580	574	10
5	830	828	2
6	362	363	-4
7	186	174	44
8	335	331	12
9	488	479	18
10	316	316	0
11	92	94	-4
12	241	242	-3
13	145	144	1
14	278	277	1
15	82	83	-2
16	147	150	-8
17	68	70	-5
18	211	203	20
19	116	116	0
20	70	66	8

1 5 1

0	274	265	32

1	388	394	-14
2	202	208	-21
3	147	153	-21
4	192	197	-18
5	197	205	-29
6	190	194	-11
7	257	255	6
8	334	342	28
9	187	179	24
10	81	91	-30
11	108	113	-15
12	177	170	21
13	80	79	4
14	88	101	-36
15	358	346	27
16	253	243	24
17	156	158	-5
18	116	123	-17
19	79	89	-22

1 7 1

0	141	137	20
1	329	316	35
2	205	207	-6
3	154	158	-4
4	114	107	21
5	385	378	17
6	84	81	8
7	272	265	20
8	303	299	11
9	197	199	-6
10	96	87	23
11	170	168	7
12	71	71	0
13	123	121	5
14	110	99	28
15	74	83	-20
16	79	80	-1
17	69	61	15

1 9 1

0	54	54	1
1	207	199	22
2	188	194	-19
3	206	212	-17
4	133	127	16
5	313	316	-6
6	143	142	1
7	224	223	1
8	166	153	36
9	225	231	-15
10	126	117	24
11	215	210	14
12	77	64	24
13	85	88	-6
14	147	143	8
15	173	162	26

1 11 1

0	45	51	-15
1	166	158	21
2	99	97	4
3	114	119	-11
4	92	89	6
5	99	101	-4
6	61	65	-7
7	157	161	-11
8	143	142	2
9	82	80	3
10	77	71	10
11	127	133	-14
12	121	122	-1

1 13 1

0	124	115	29
1	-16	23	-15
2	23	26	-2
3	-10	29	-17
4	88	79	18
5	-25	16	-16

2 0 1

0	751	720	47
2	954	949	4
4	877	890	-15
6	952	937	15
8	746	712	42
10	504	486	29
12	113	109	9
14	236	229	13
16	147	147	0
18	112	119	-11
20	127	121	9

2 2 1

0	674	667	13
1	827	836	-12
2	841	839	2
3	68	56	41
4	409	417	-21
5	364	362	4
6	424	433	-23
7	98	94	12
8	355	361	-16
9	400	387	32
10	226	218	24
11	84	95	-34
12	153	155	-5
13	222	223	0
14	141	135	17
15	207	210	-7
16	90	84	13
17	106	109	-7
18	45	41	6
19	26	49	-31
20	82	84	-5

2 4 1

0	227	226	2
1	877	892	-18
2	471	465	12
3	177	185	-30
4	94	100	-19
5	460	478	4
6	552	540	23
7	533	526	13
8	326	327	-2
9	235	228	19
10	139	137	6
11	287	290	-6
12	20	6	8
13	361	348	30
14	93	96	-6
15	78	74	7
16	131	131	1
17	238	230	19
18	85	84	0
19	90	87	5

2 6 1

0	574	573	2
1	513	525	-25
2	847	860	-17
3	848	829	24
4	250	241	27
5	124	125	-3
6	212	202	30
7	406	395	25
8	157	160	-10
9	319	312	17
10	154	153	2
11	172	161	29
12	25	41	-21
13	98	98	0
14	210	209	1
15	82	84	-4
16	-13	12	-6
17	125	120	10
18	31	39	-10

2 8 1

0	191	186	19
1	143	147	-12
2	155	153	9
3	27	27	0
4	148	152	-13
5	65	56	20
6	279	277	6
7	80	79	2
8	208	206	1
9	22	28	-7
10	122	124	-4
11	10	29	-15
12	150	149	2
13	135	141	-15
14	68	61	12
15	116	118	-4
16	181	172	20

2 10 1

0	96	87	30
1	177	178	-3
2	40	33	9
3	97	103	-17
4	98	89	21
5	86	91	-12
6	77	71	12
7	93	104	-22
8	79	90	-27
9	104	105	-4
10	16	10	3
11	46	38	10
12	93	105	-26
13	78	80	-2

2 12 1

0	60	62	-5
1	24	26	-1
2	48	43	6
3	85	85	1
4	19	24	-4
5	28	44	-20
6	51	43	11
7	61	60	0
8	-32	4	-20

3 1 1

0	593	595	-4
1	843	840	3
2	126	121	20
3	500	505	-10
4	130	140	-42
5	190	194	-17
6	-46	6	-72
7	510	497	27
8	289	291	-8
9	152	137	48
10	107	110	-10
11	372	363	20
12	66	65	0
13	239	242	-7
14	32	38	-5
15	163	159	11
16	113	110	6
17	144	139	12
18	26	11	10
19	92	80	24
20	46	48	-2

3 3 1

0	498	516	-45
1	146	146	-1
2	247	250	-10
3	74	84	-38
4	264	270	-21
5	437	450	-30
6	308	299	27
7	126	126	2
8	344	340	9
9	381	370	27
10	190	173	52
11	80	77	7
12	243	247	-11
13	126	120	15
14	177	177	0
15	39	33	8
16	96	92	8
17	124	129	-11
18	108	111	-7
19	10	23	-8

3 5 1

0	411	416	-14
1	248	241	20
2	509	501	15
3	279	275	12
4	82	73	29
5	19	18	0
6	301	301	0
7	64	76	-36
8	204	207	-8
9	57	61	-10
10	158	146	34
11	176	174	7
12	234	227	18
13	65	68	-4
14	76	78	-4
15	140	149	-22
16	189	204	-39
17	35	46	-14
18	93	84	19

3 7 1

0	226	217	34
1	135	130	13
2	207	212	-17
3	435	436	-1
4	160	169	-31
5	67	67	0
6	97	98	-1
7	283	288	-15
8	103	101	5
9	148	149	-4
10	63	72	-22
11	189	189	-1
12	95	104	-22
13	118	113	13
14	108	105	7
15	106	107	-3
16	25	34	-10
17	108	105	7

3 9 1

0	217	224	-26
1	394	399	-11
2	337	336	2

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3	238	243	-14
4	199	202	-7
5	306	306	1
6	90	82	18
7	189	184	13
8	9	16	-3
9	88	91	-5
10	31	36	-6
11	34	40	-8
12	7	12	-2
13	103	100	7
14	43	39	5

3 11 1

0	72	66	18
1	25	26	-1
2	50	60	-18
3	69	66	6
4	120	122	-4
5	102	100	4
6	45	50	-9
7	74	74	-1
8	83	80	6
9	-24	26	-24
10	12	17	-2

3 13 1

0	91	80	29
1	50	57	-11

4 0 1

0	773	773	0
2	637	636	0
4	231	233	-5
6	183	185	-5
8	109	114	-10
10	147	157	-25
12	266	267	0
14	168	161	14
16	232	236	-8
18	42	50	-9

4 2 1

0	331	331	0
1	225	227	-7
2	370	356	36
3	73	95	-77
4	273	285	-38
5	96	97	-5
6	225	214	33
7	363	361	6
8	114	111	8
9	115	112	8
10	215	217	-4
11	112	119	-22
12	97	93	9
13	80	77	8
14	114	122	-24
15	215	209	14
16	-18	5	-7
17	33	52	-30
18	102	100	6
19	41	61	-32

4 4 1

0	295	293	6
1	353	348	12
2	371	384	-36
3	243	233	31
4	234	236	-7
5	192	193	-4
6	220	220	-1
7	179	178	1
8	63	69	-17
9	257	231	26
10	113	118	-15
11	168	174	-19
12	110	107	7
13	64	80	-38
14	93	98	-13
15	102	98	9
16	53	55	-4
17	33	36	-3
18	-22	35	-33

4 6 1

0	121	121	-3
1	89	94	-14
2	84	95	-37
3	85	87	-6
4	97	96	5
5	164	168	-15
6	209	202	20
7	242	240	4
8	146	145	2
9	143	130	35
10	172	177	-15
11	83	92	-23
12	113	112	5
13	109	119	-26
14	68	71	-7
15	16	33	-16
16	47	53	-9
17	32	47	-19

4 8 1

0	207	199	30
1	81	83	-4
2	225	228	-9
3	92	99	-20
4	120	124	-10
5	171	178	-21
6	282	272	27
7	75	73	4
8	100	99	1
9	28	33	-6
10	164	163	2
11	-15	5	-5
12	69	69	1
13	22	22	0
14	63	59	7
15	-25	10	-13

4 10 1

0	149	148	3
1	55	50	8
2	159	158	0
3	49	56	-12
4	299	303	-9
5	223	212	28
6	199	201	-6
7	119	120	-3
8	217	219	-4
9	199	192	18
10	33	25	7
11	-18	21	-14
12	12	49	-38

4 12 1

0	119	121	-8
1	205	210	-10
2	111	120	-22
3	105	112	-17
4	103	111	-18
5	166	168	-5
6	69	71	-4

5 1 1

0	475	448	65
1	812	795	28
2	745	734	16
3	514	501	26
4	116	118	-7
5	469	470	-1
6	136	132	11
7	296	304	-22
8	91	95	-12
9	342	337	12
10	82	87	-12
11	208	211	-8
12	60	65	-12
13	342	345	-8
14	131	137	-16
15	97	90	18
16	83	87	-9
17	180	188	-22
18	51	51	0
19	61	60	1

5 3 1

0	195	195	0
1	132	138	-21
2	345	341	9
3	208	215	-26
4	201	201	0
5	200	201	-3
6	171	168	9
7	223	225	-6
8	172	165	22
9	157	159	-6
10	139	139	0
11	71	92	-58
12	174	166	22
13	20	29	-9
14	114	117	-7
15	106	115	-23
16	127	128	-1
17	-12	34	-25
18	17	42	-26

5 5 1

0	218	218	0
1	99	102	-9
2	222	213	26
3	43	42	3
4	190	182	23
5	40	47	-14
6	244	256	-36
7	80	84	-11
8	234	229	14
9	-19	25	-25
10	177	179	-3
11	71	67	8
12	57	55	5
13	59	66	-13
14	100	98	6
15	-5	36	-25
16	34	41	-10
17	8	24	-8

5 7 1

0	138	143	-19
1	69	68	3
2	154	158	-13
3	262	262	-1
4	172	165	19
5	197	197	0
6	401	404	-7
7	404	401	6
8	180	177	7
9	285	283	4
10	160	168	-20
11	134	143	-22
12	-24	14	-16
13	93	94	-1
14	49	45	5
15	71	63	14

5 9 1

0	82	91	-31
1	146	146	1
2	73	81	-19
3	202	198	10
4	28	13	12
5	100	99	1
6	27	35	-9
7	215	213	5
8	71	71	0
9	103	98	11
10	53	60	-12
11	139	137	4
12	76	74	2

5 11 1

0	9	25	-15
1	50	51	0
2	110	104	13
3	78	89	-24
4	59	67	-15
5	130	134	-9
6	94	96	-4
7	26	5	11
8	28	28	0

6 0 1

0	448	436	26
2	190	184	15
4	194	188	12
6	254	241	27
8	329	328	2
10	164	170	-12
12	249	252	-7
14	194	201	-14
16	174	189	-28
18	106	109	-5

6 2 1

0	408	408	-1
1	155	145	34
2	257	243	42
3	238	238	0
4	282	284	-6
5	278	278	-1
6	80	79	1
7	158	158	0
8	261	263	-5
9	135	130	14
10	83	84	0
11	129	130	-2
12	139	139	0
13	126	126	0
14	148	150	-5
15	85	90	-12
16	67	74	-13
17	85	83	4

6 4 1

0	154	153	2
1	341	341	0
2	130	131	-3
3	326	336	-26
4	211	208	9
5	209	212	-8
6	286	295	-24

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7	543	541	3
8	331	325	14
9	176	183	-21
10	168	179	-33
11	263	270	-19
12	96	105	-23
13	119	100	45
14	50	38	18
15	-13	22	-13
16	42	39	3
17	112	111	3

6 6 1

0	163	161	5
1	157	150	20
2	109	109	0
3	170	180	-30
4	119	117	5
5	218	219	-4
6	159	149	29
7	139	142	-9
8	46	48	-4
9	122	119	5
10	145	143	5
11	50	56	-12
12	48	59	-19
13	29	48	-27
14	54	54	0
15	80	71	17

6 8 1

0	121	120	1
1	-33	18	-35
2	132	127	13
3	36	39	-4
4	167	169	-5
5	130	127	7
6	134	132	3
7	82	85	-8
8	146	154	-22
9	106	108	-4
10	51	51	0
11	42	53	-11
12	93	88	11
13	-38	0	-29

6 10 1

0	55	58	-8
1	71	65	12
2	59	61	-3
3	44	42	3
4	44	46	-3
5	50	37	17
6	78	76	3
7	91	91	1
8	68	68	-1
9	-21	16	-13

7 1 1

0	257	262	-18
1	267	269	-6
2	64	53	26
3	77	82	-13
4	182	185	-11
5	249	249	-2
6	307	304	9
7	226	219	21
8	424	418	13
9	329	321	19
10	272	266	15
11	108	108	0
12	112	118	-17
13	115	120	-13
14	11	25	-10
15	46	56	-16
16	29	41	-13

7 3 1

0	349	357	-22
1	220	217	7
2	211	214	-10
3	91	96	-16
4	200	200	1
5	271	272	-2
6	334	327	17
7	126	129	-10
8	163	159	9
9	108	104	12
10	150	147	8
11	143	142	1
12	183	176	19
13	21	32	-11
14	121	116	12
15	80	88	-18
16	44	47	-5

7 5 1

0	436	443	-17
1	266	269	-7
2	201	197	10
3	98	92	16
4	497	495	4
5	57	38	33
6	111	102	24
7	173	171	7
8	384	371	27
9	89	81	18
10	168	156	29
11	19	9	5
12	179	177	4
13	62	51	19
14	106	113	-16
15	73	63	17

7 7 1

0	104	100	14
1	117	120	-10
2	191	192	-3
3	20	19	0
4	112	111	2
5	124	127	-8
6	117	122	-14
7	78	78	0
8	99	100	-1
9	89	92	-6
10	47	50	-5
11	20	26	-4
12	136	128	19
13	123	116	14

7 9 1

0	91	81	29
1	74	72	4
2	78	82	-8
3	62	66	-7
4	25	32	-7
5	63	68	-8
6	30	31	-1
7	35	42	-8
8	-24	23	-21
9	29	36	-7

7 11 1

0	58	61	-9
1	51	47	6

8 0 1

0	169	167	7
2	170	173	-7
4	175	175	0
6	132	143	-24
8	193	192	2
10	103	98	7
12	121	123	-3
14	109	118	-15

8 2 1

0	110	113	-12
1	119	111	23
2	8	27	-16
3	83	89	-16
4	31	20	13
5	325	323	7
6	175	175	-1
7	207	202	14
8	144	132	32
9	393	390	7
10	210	213	-6
11	119	127	-21
12	52	57	-9
13	102	101	2
14	98	103	-10
15	56	59	-4

8 4 1

0	100	106	-26
1	127	131	-14
2	73	80	-17
3	74	75	-3
4	94	90	8
5	116	124	-24
6	90	89	1
7	133	134	-2
8	48	52	-6
9	123	112	29
10	98	96	3
11	89	84	9
12	106	103	8
13	166	161	10
14	34	37	-3

8 6 1

0	111	113	-10
1	121	127	-16
2	71	80	-23
3	67	75	-18
4	104	110	-18
5	56	64	-15
6	27	30	-2
7	38	38	0
8	64	66	-4
9	69	74	-8
10	62	60	4
11	113	111	5
12	-11	16	-7

8 8 1

0	-28	23	-42
1	58	65	-15
2	150	156	-17
3	93	105	-30
4	23	27	-3
5	35	56	-33
6	95	99	-9
7	50	61	-18
8	56	54	3
9	-25	17	-17

8 10 1

0	89	84	12
1	29	36	-7
2	51	58	-12

9 1 1

0	48	56	-22
1	142	135	19
2	-19	16	-15
3	104	108	-12
4	83	82	3
5	65	69	-8
6	131	127	8
7	220	227	-19
8	60	68	-16
9	28	39	-14
10	104	105	-2
11	139	141	-5
12	35	37	-2
13	30	40	-12

9 3 1

0	41	50	-23
1	159	166	-19
2	148	151	-6
3	35	40	-7
4	124	128	-11
5	86	84	4
6	32	38	-7
7	70	76	-14
8	97	92	11
9	14	11	1
10	88	87	4
11	41	33	10
12	30	38	-8
13	-32	17	-25

9 5 1

0	137	147	-37
1	70	76	-11
2	71	66	10
3	19	44	-31
4	113	120	-20
5	104	101	6
6	22	23	0
7	156	146	25
8	151	151	-1
9	152	157	-12
10	94	100	-13
11	125	117	17

9 7 1

0	112	111	2
1	48	48	-1
2	13	24	-8
3	53	60	-12
4	59	55	8
5	29	34	-6
6	52	58	-10
7	22	34	-12
8	-18	22	-15

9 9 1

0	49	47	5
1	28	37	-9
2	-28	5	-15

10 0 1

0	253	261	-20
2	183	185	-3
4	90	89	1
6	81	72	14
8	-33	22	-24

I-1147-1147

10	-30	22	-19

10	2	1	
0	89	88	5
1	79	91	-28
2	19	41	-27
3	19	42	-28
4	-26	19	-23
5	82	84	-4
6	53	54	-1
7	75	78	-6
8	-17	25	-18
9	-32	22	-32
10	-35	14	-29
11	12	30	-13

10	4	1	
0	31	46	-30
1	120	128	-21

2	24	16	7
3	98	102	-10
4	32	28	4
5	110	111	-1
6	51	53	-3
7	81	82	-2
8	52	52	0
9	119	119	-2
10	30	55	-24

10	6	1	
0	51	44	14
1	75	67	14
2	19	9	5
3	60	59	1
4	18	20	-1
5	50	50	0
6	77	75	2
7	51	53	-3

11	1	1	
0	17	30	-17
1	30	33	-3
2	41	52	-18
3	112	115	-7
4	-23	22	-20
5	48	49	-1
6	35	49	-20
7	6	30	-15
8	22	40	-19

11	3	1	
0	122	116	19
1	114	112	4
2	44	43	1
3	53	47	9
4	84	91	-14
5	47	52	-7
6	84	83	3

7	-33	16	-27

11	5	1	
0	49	44	9
1	-21	12	-12
2	68	77	-16
3	-1	27	-13
4	67	72	-10

12	0	1	
0	-19	28	-21
2	89	81	10

12	2	1	
0	22	25	-3
1	57	57	0
2	45	60	-24

I-1147-m48

Table S4E. Observed and Calculated Structure Factors for 4′-Methoxy-N-methyl-4-stilbazolium Tosylate

The columns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

I-1147-m49

-11 0 1

1	57	57	0
2	65	69	-28
3	35	31	40
4	36	34	14
5	30	36	-62

-10 0 1

1	-10	2	-15
2	29	33	-43
3	42	48	-64
4	34	36	-24
5	7	8	-7
6	62	64	-19
7	22	27	-52
8	7	13	-29
9	-10	13	-41

-9 0 1

1	75	78	-17
2	12	15	-15
3	14	14	-1
4	108	109	-5
5	21	17	36
6	181	179	7
7	20	5	82
8	11	14	-8
9	8	16	-50
10	23	27	-36
11	38	41	-36
12	56	53	9

-8 0 1

1	44	42	23
2	294	302	-25
3	51	44	64
4	53	55	-25
5	20	3	88
6	234	238	-14
7	116	116	-3
8	21	23	-17
9	42	43	-9
10	65	63	15
11	4	4	0
12	32	35	-34
13	65	61	28

-7 0 1

1	63	60	21
2	15	17	-10
3	26	26	-5
4	204	209	-21
5	230	228	8
6	161	162	-4
7	52	52	0
8	62	60	11
9	6	5	1
10	82	82	0
11	88	82	34
12	42	38	44
13	41	41	-5
14	59	59	6
15	-11	1	-18

-6 0 1

1	249	257	-30
2	194	200	-27
3	71	65	39
4	76	82	-49
5	172	172	0
6	132	142	-53
7	29	31	-17
8	74	68	37
9	91	89	15
10	24	24	-2
11	10	10	3
12	110	109	6
13	82	52	70
14	46	53	-71
15	8	12	-22
16	44	44	2

-5 0 1

1	75	70	34
2	147	145	9
3	50	60	-84
4	-6	19	-64
5	142	135	40
6	25	20	38
7	28	33	-59
8	25	31	-44
9	66	74	-61
10	21	21	-1
11	75	70	31
12	32	36	-50
13	109	101	43
14	-5	0	-3
15	3	10	-10
16	5	9	-9
17	51	49	19

-4 0 1

1	257	276	-72
2	169	154	73
3	20	21	-16
4	98	106	-63
5	102	87	93
6	179	159	91
7	18	20	-16
8	137	135	10
9	74	75	-8
10	152	136	76
11	106	87	103
12	137	132	23
13	20	22	-24
14	72	71	10
15	12	14	-13
16	32	29	28
17	-14	4	-37

-3 0 1

1	372	371	4
2	149	161	-76
3	46	31	108
4	52	52	2
5	42	30	105
6	144	151	-42
7	60	69	-74
8	18	20	-13
9	205	206	-4
10	30	35	-33
11	112	123	-65
12	94	83	59
13	99	92	37
14	61	69	-62
15	-9	13	-35
16	25	26	-9
17	41	38	25
18	-11	1	-18

-2 0 1

1	1048	1150	-101
2	370	378	-20
3	94	89	35
4	241	253	-49
5	92	91	3
6	54	57	-25
7	41	35	54
8	253	258	-16
9	88	78	68
10	154	142	61
11	108	102	32
12	109	115	-32
13	167	160	33
14	36	34	26
15	30	32	-16
16	32	33	-5
17	14	17	-27
18	28	28	-5

-1 0 1

1	109	113	-32
2	87	76	76
3	75	72	18
4	373	388	-38
5	108	107	9
6	391	401	-26
7	40	43	-34
8	69	68	2
9	93	100	-54
10	82	83	-11
11	8	14	-11
12	197	198	-1
13	28	29	-10
14	91	84	35
15	-11	12	-37
16	53	55	-17
17	17	19	-13
18	-2	5	-4

0 0 1

2	319	318	3
3	43	31	82
4	689	714	-41
5	264	261	12
6	36	36	0
7	197	191	35
8	129	123	45
9	62	60	15
10	78	80	-26
11	217	225	-38
13	167	169	-7
14	85	89	-26
15	74	80	-46
16	29	23	5
17	33	29	46
18	48	50	-27

1 0 1

0	89	81	63
1	129	120	56
2	144	133	62
3	154	170	-95
4	199	206	-29
5	341	346	-14
6	137	143	-36
7	89	87	12
8	182	173	39
9	130	123	39
10	13	13	1
11	110	118	-49
12	179	182	-14
13	192	182	41
14	14	12	7
15	9	0	9
16	65	72	-58
17	32	28	36
18	39	31	83

2 0 1

0	1016	1109	-95
1	421	429	-21
2	46	48	-11
3	165	166	-14
4	27	31	-28
5	10	4	15
6	94	98	-32
7	92	94	-13
8	25	25	-7
9	105	104	3
10	101	101	1
11	101	111	-64
12	103	103	0
13	171	178	-33
14	92	99	-37
15	21	27	-55
16	-3	7	-16
17	53	56	-30
18	30	35	-51

3 0 1

0	688	716	-40
1	29	35	-41
2	15	20	-21
3	344	323	60
4	38	44	-66
5	248	253	-19
6	86	86	-1
7	45	42	29
8	128	138	-64
9	-8	9	-41
10	-7	4	-7
11	189	187	9
12	36	29	79
13	121	113	41
14	43	44	-14
15	49	51	-22
16	54	52	15
17	5	3	3
18	25	23	14

4 0 1

0	102	98	26
1	83	86	-24
2	18	14	38
3	178	156	102
4	339	311	76
5	22	15	57
6	10	7	8
7	110	120	-61
8	112	104	50
9	74	70	28
10	77	79	-13
11	15	13	18
12	130	126	25
13	47	48	-4
14	25	26	-4
15	-10	9	-23
16	53	54	-6
17	20	19	6

5 0 1

0	290	299	-29
1	64	48	108
2	82	87	-38
3	236	229	28
4	215	212	14
5	134	140	-39
6	36	38	-25
7	-9	5	-10
8	111	115	-21
9	21	14	50
10	30	24	60
11	93	87	39

12	32	34	-22
13	27	29	-18
14	-6	6	-23
15	42	37	47
16	68	65	18

6 0 l

0	137	128	51
1	-6	5	-12
2	134	142	-51
3	117	99	100
4	64	45	102
5	19	31	-73
6	138	134	18
7	35	33	14
8	110	102	48
9	75	68	41
10	79	70	49
11	61	59	14
12	41	39	21
13	20	18	11
14	32	25	66
15	42	42	0

7 0 l

0	133	128	24
1	22	17	42
2	8	11	-9
3	91	84	44
4	125	117	45
5	-8	1	-12
6	15	19	-19
7	157	148	43
8	28	21	67
9	-11	4	-19
10	48	49	-5
11	42	34	78
12	35	38	-24
13	13	18	-35
14	15	14	4

8 0 l

0	77	79	-11
1	105	104	10
2	80	76	26
3	15	17	-13
4	30	32	-21
5	94	88	38
6	92	83	46
7	38	41	-29
8	125	128	-16
9	39	34	52
10	19	11	51
11	35	40	-63
12	57	56	8
13	30	29	11

9 0 l

0	39	39	3
1	3	17	-32
2	71	74	-20
3	60	57	17
4	-13	1	-25
5	13	9	20
6	43	41	23
7	53	48	42
8	17	16	12
9	3	17	-40
10	48	46	18
11	38	37	3

10 0 l

0	21	24	-28
1	51	53	-21
2	-15	2	-29
3	7	19	-34
4	21	24	-34
5	54	53	2
6	34	28	55
7	115	116	-6
8	34	35	-12

11 0 l

0	-6	1	-7
1	13	19	-44
2	21	27	-62
3	19	23	-36
4	-16	5	-48

-11 1 l

1	19	19	8
2	28	32	-50
3	16	19	-32
4	-6	14	-53

-10 1 l

1	96	98	-16
2	51	49	22
3	33	35	-23
4	16	19	-37
5	40	42	-23
6	39	40	-15
7	17	22	-66
8	53	56	-37
9	9	13	-30

-9 1 l

1	46	45	16
2	123	120	20
3	115	113	10
4	25	21	44
5	38	39	-10
6	80	83	-18
7	43	44	-14
8	13	19	-61
9	15	12	25
10	80	77	31
11	44	43	5

-8 1 l

1	111	107	35
2	167	168	-5
3	77	77	-6
4	70	68	14
5	15	19	-41
6	45	45	-7
7	60	61	-18
8	79	82	-24
9	57	56	9
10	100	100	0
11	60	59	0
12	31	27	46
13	52	51	10

-7 1 l

1	158	160	-13
2	189	193	-18
3	99	102	-20
4	25	22	36
5	138	139	-6
6	192	191	5
7	42	40	40
8	66	69	-35
9	123	120	21
10	126	123	18
11	30	24	69
12	99	101	-11
13	30	28	19
14	27	27	-2
15	30	31	-19

-6 1 l

1	183	182	6
2	124	128	-33
3	75	80	-49
4	94	97	-30
5	25	19	45
6	46	42	37
7	104	105	-9
8	76	72	29
9	82	80	10
10	87	86	5
11	70	66	38
12	21	20	1
13	62	58	38
14	31	29	29
15	-6	11	-52
16	7	13	-40

-5 1 l

1	292	286	22
2	40	40	1
3	25	21	49
4	36	38	-26
5	202	213	-59
6	69	54	125
7	102	92	74
8	55	50	52
9	104	102	16
10	34	35	-22
11	83	77	49
12	125	119	38
13	38	42	-70
14	41	41	0
15	62	58	37
16	63	59	39
17	-8	2	-16

-4 1 l

1	268	259	33
2	68	73	-56
3	180	186	-39
4	89	93	-40
5	190	184	31
6	143	131	78
7	92	92	-6
8	52	56	-48
9	70	64	52
10	87	79	65
11	55	57	-21
12	68	64	33
13	64	58	50
14	14	14	5
15	-6	9	-22
16	15	16	-12
17	41	38	48

-3 1 l

1	496	478	39
2	189	188	4
3	55	60	-54
4	168	172	-28
5	233	242	-46
6	226	209	78
7	45	44	4
8	95	104	-82
9	50	46	40
10	65	63	18
11	121	115	43
12	91	90	10
13	126	128	-8
14	72	72	7
15	54	50	42
16	24	20	47
17	27	26	5
18	65	66	-4

-2 1 l

1	244	244	0
2	331	337	-20
3	179	176	18
4	91	91	2
5	237	217	92
6	241	242	-2
7	59	61	-17
8	108	99	70
9	81	83	-20
10	140	146	-41
11	50	46	35
12	64	58	48
13	44	43	10
14	26	26	2
15	30	28	16
16	67	66	13
17	25	22	37
18	26	25	19

-1 1 l

1	395	402	-21
2	282	298	-65
3	196	193	15
4	903	956	-69
5	441	454	-33
6	98	90	66
7	147	148	-8
8	225	220	24
9	22	21	9
10	131	128	22
11	164	168	-18
12	43	45	-34
13	90	89	7
14	105	103	17
15	14	18	-32
16	21	21	-8
17	57	51	75
18	87	84	31

0 1 l

1	448	472	-62
2	506	534	-68
3	404	411	-22
4	825	879	-85
5	263	257	25
6	195	194	1
7	124	113	99
8	271	272	-3
9	85	90	-52
10	151	149	15
11	46	47	-9
12	104	111	-71
13	43	47	-67
14	61	60	10
15	69	66	32
16	80	80	0
17	13	13	-5
18	15	14	9

1 1 l

0	528	551	-47
1	390	398	-22
2	86	80	55
3	731	769	-60
4	893	948	-73

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5	208	207	6
6	303	289	48
7	243	242	6
8	152	145	43
9	162	156	37
10	244	246	-12
11	101	106	-41
12	67	69	-22
13	84	88	-31
14	103	103	1
15	13	19	-66
16	-4	8	-15
17	76	78	-11
18	63	64	-6

2 1 1

0	248	243	20
1	608	637	-55
2	243	245	-11
3	418	404	36
4	211	200	55
5	123	125	-13
6	151	146	35
7	205	194	56
8	129	132	-21
9	108	103	38
10	91	90	12
11	41	46	-66
12	118	126	-63
13	54	52	24
14	73	72	10
15	52	57	-60
16	31	31	0
17	37	38	-14
18	33	31	25

3 1 1

0	149	146	24
1	353	360	-23
2	115	115	-3
3	128	131	-21
4	-3	7	-38
5	46	44	20
6	171	170	8
7	58	60	-42
8	154	147	43
9	145	147	-11
10	117	117	1
11	5	12	-22
12	93	91	17
13	109	113	-26
14	11	17	-44
15	22	19	30
16	53	53	-7
17	75	76	-4

4 1 1

0	122	128	-51
1	355	351	12
2	124	115	63
3	101	99	17
4	116	125	-76
5	67	67	-4
6	116	117	-9
7	90	88	18
8	161	157	27
9	54	56	-15
10	27	24	38
11	60	56	39
12	98	98	-4
13	10	10	-2
14	76	74	15
15	50	49	23
16	12	14	-9
17	12	13	-9

5 1 1

0	224	211	59
1	200	196	20
2	76	78	-13
3	107	103	28
4	30	26	53
5	33	31	24
6	167	174	-40
7	96	83	93
8	105	97	64
9	49	45	38
10	59	57	24
11	47	50	-32
12	142	136	32
13	34	31	48
14	72	75	-30
15	15	21	-60
16	57	54	37

6 1 1

0	316	315	3
1	73	75	-19
2	86	81	45
3	40	42	-25
4	102	101	2
5	46	48	-24
6	60	62	-23
7	129	118	72
8	86	85	13
9	42	42	-10
10	35	31	46
11	64	57	64
12	98	94	25
13	71	66	39
14	75	73	25
15	35	32	38

7 1 1

0	72	64	70
1	167	161	35
2	124	125	-1
3	65	62	27
4	37	38	-3
5	116	112	23
6	94	88	48
7	31	36	-76
8	51	50	6
9	75	67	58
10	50	43	81
11	39	40	-2
12	113	107	43
13	43	49	-54
14	32	33	-18

8 1 1

0	194	190	18
1	99	100	-6
2	106	110	-31
3	31	28	49
4	79	78	4
5	42	47	-57
6	78	78	-2
7	59	53	50
8	53	50	32
9	17	21	-48
10	29	28	8
11	55	51	43
12	7	5	5

9 1 1

0	88	91	-20
1	98	98	-1
2	52	49	36
3	32	39	-118
4	61	66	-54
5	52	47	47
6	40	37	37
7	29	33	-51
8	82	83	-2
9	36	35	15
10	14	10	22

10 1 1

0	37	38	-11
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2	-5	4	-8
3	48	50	-36
4	43	44	-25
5	39	43	-64
6	42	45	-40
7	9	12	-23
8	14	19	-42

11 1 1

0	58	64	-67
1	2	6	-7
2	37	38	-18
3	4	13	-51

-10 2 1

1	33	37	-63
2	42	42	-1
3	31	27	58
4	-6	12	-75
5	9	13	-26
6	43	41	25
7	31	28	40
8	32	29	41

-9 2 1

1	28	26	26
2	34	39	-89
3	26	29	-45
4	54	49	55
5	44	43	2
6	-9	3	-31
7	36	39	-49
8	33	30	38
9	-4	9	-30
10	18	21	-33

-8 2 1

1	84	85	-11
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3	84	81	27
4	9	13	-20
5	77	75	18
6	67	63	31
7	34	33	21
8	40	43	-42
9	60	58	19
10	72	69	24
11	17	20	-36
12	24	25	-8

-7 2 1

1	92	91	11
2	56	52	35
3	90	85	39
4	90	86	34
5	66	63	33
6	53	56	-30
7	109	101	54
8	44	39	59
9	40	42	-30
10	42	45	-42
11	68	66	23
12	85	83	14
13	78	73	46
14	87	84	21

-6 2 1

1	132	131	3
2	103	106	-19
3	11	6	20
4	51	53	-24
5	68	68	6
6	97	96	10
7	47	54	-91
8	91	94	-17
9	86	83	25
10	77	76	8
11	78	77	5
12	43	42	21
13	61	57	43
14	33	27	78
15	16	17	-6

-5 2 1

1	140	132	54
2	84	81	24
3	199	200	-5
4	185	181	20
5	98	86	95
6	100	99	7
7	177	174	16
8	25	23	17
9	47	48	-18
10	88	83	37
11	47	46	9
12	97	90	46
13	69	66	20
14	46	42	47
15	19	17	20
16	15	15	4

-4 2 1

1	369	369	2
2	203	184	96
3	146	142	27
4	117	109	60
5	187	184	14
6	65	72	-69
7	203	195	37
8	112	112	-3
9	18	23	-78
10	16	20	-55
11	75	72	24
12	62	59	29
13	13	19	-42
14	64	65	-9
15	76	72	27
16	42	39	47
17	30	33	-35

-3 2 1

1	153	140	79
2	117	122	-41
3	298	300	-8
4	115	113	18
5	71	69	17
6	210	211	-6
7	98	107	-80
8	86	83	21
9	63	64	-10
10	92	94	-15
11	-1	8	-25
12	44	45	-21

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13	80	78	15
14	43	40	41
15	61	59	17
16	65	66	-7
17	24	20	50

-2 2 1

1	156	155	3
2	159	161	-10
3	133	129	27
4	84	87	-31
5	145	148	-23
6	18	11	70
7	290	285	18
8	104	105	-11
9	98	97	10
10	25	25	1
11	86	85	3
12	56	55	14
13	39	42	-57
14	111	107	26
15	121	116	32
16	31	28	53
17	56	56	3
18	87	81	45

-1 2 1

1	276	291	-62
2	113	124	-100
3	115	121	-54
4	195	184	59
5	164	163	6
6	236	231	26
7	192	177	78
8	266	254	49
9	97	91	50
10	44	47	-34
11	26	28	-41
12	150	152	-13
13	51	51	-2
14	111	107	25
15	55	54	16
16	66	68	-21
17	38	36	26
18	19	16	30

0 2 1

0	279	286	-26
1	109	109	-3
2	113	103	97
3	261	268	-33
4	244	241	17
5	211	206	24
6	367	349	62
7	428	433	-16
8	344	354	-39
9	144	138	47
10	101	99	25
11	90	91	-8
12	99	98	15
13	45	47	-38
14	66	67	-15
15	37	38	-28
16	20	20	-12
17	44	42	36
18	34	33	27

1 2 1

0	284	279	19
1	178	186	-50
2	157	173	-115
3	187	179	45
4	183	172	66
5	142	139	21
6	392	387	15
7	357	343	42
8	313	301	40
9	69	62	67
10	97	104	-57
11	92	99	-62
12	118	124	-39
13	48	46	23
14	34	38	-59
15	41	42	-16
16	47	46	15
17	25	25	0
18	55	51	51

2 2 1

0	320	318	9
1	167	162	29
2	68	62	56
3	107	109	-12
4	145	151	-48
5	286	278	48
6	342	324	57
7	239	245	-31
8	183	180	15
9	74	75	-8
10	98	98	0
11	82	78	27
12	34	38	-66
13	61	68	-66
14	52	51	4
15	16	19	-37
16	16	21	-64
17	47	45	27

3 2 1

0	124	129	-36
1	338	334	12
2	117	120	-22
3	71	69	21
4	72	79	-78
5	209	209	0
6	152	140	73
7	130	124	38
8	52	59	-78
9	70	71	-6
10	30	25	60
11	75	76	-8
12	115	117	-18
13	36	35	12
14	13	20	-74
15	28	28	-6
16	23	23	-7
17	15	16	-4

4 2 1

0	162	160	12
1	43	42	9
2	87	95	-79
3	122	125	-23
4	26	30	-63
5	146	142	27
6	158	155	14
7	51	48	25
8	47	49	-24
9	105	106	-10
10	14	16	-20
11	89	90	-7
12	105	107	-12
13	90	87	21
14	5	5	0
15	20	18	27
16	52	49	33

5 2 1

0	158	165	-48
1	149	160	-73
2	116	101	111
3	60	55	46
4	130	132	-15
5	23	25	-14
6	96	88	60
7	85	82	22
8	119	119	0
9	108	108	-2
10	119	120	-8
11	127	119	55
12	57	56	15
13	79	78	3
14	54	52	21
15	10	12	-18

6 2 1

0	39	41	-19
1	178	172	33
2	169	173	-23
3	98	96	15
4	32	25	100
5	155	146	54
6	57	56	10
7	19	22	-38
8	100	97	25
9	110	111	-5
10	86	90	-30
11	37	35	21
12	94	91	25
13	47	45	33
14	24	26	-28

7 2 1

0	91	91	0
1	60	55	45
2	78	86	-72
3	18	15	33
4	72	70	17
5	36	34	37
6	98	97	8
7	49	48	12
8	80	81	-9
9	73	73	1
10	89	86	23
11	72	73	-15
12	48	48	8
13	25	27	-22

8 2 1

0	73	71	16
1	194	191	17
2	205	201	18
3	33	30	48
4	101	103	-9
5	95	92	20
6	82	78	30
7	31	29	28
8	60	61	-11
9	13	14	-7
10	23	24	-12
11	23	23	4
12	35	36	-9

9 2 1

0	57	55	19
1	44	47	-31
2	43	44	-16
3	33	26	84
4	66	63	23
5	36	36	0
6	62	64	-25
7	42	41	24
8	9	13	-37
9	22	25	-27

10 2 1

0	102	103	-4
1	84	82	24
2	58	60	-18
3	48	53	-67
4	39	40	-13
5	27	27	-3
6	8	12	-21
7	34	33	19

-10 3 1

1	19	14	46
2	13	18	-39
3	7	13	-43
4	21	22	-7
5	49	43	74

-9 3 1

1	17	19	-14
2	37	30	81
3	18	20	-21
4	46	46	-1
5	31	31	0
6	79	75	44
7	13	13	-4
8	39	40	-12
9	9	14	-30

-8 3 1

1	24	21	41
2	22	25	-28
3	65	62	33
4	59	55	37
5	72	68	33
6	48	47	6
7	59	57	25
8	42	49	-122
9	25	26	-20
10	15	17	-23
11	20	22	-18

-7 3 1

1	77	73	29
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3	54	49	50
4	4	12	-38
5	82	78	28
6	115	106	56
7	33	38	-70
8	73	79	-55
9	47	48	-5
10	28	26	27
11	-6	12	-44
12	17	21	-36
13	51	52	-9

-6 3 1

1	81	81	0
2	74	71	29
3	92	85	50
4	100	98	16
5	50	45	52
6	152	150	12
7	39	33	75
8	55	55	-1
9	13	15	-16
10	60	58	17
11	60	59	12
12	-8	5	-15

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13	40	39	9
14	14	16	-19

-5 3 1

1	135	136	-5
2	134	135	-4
3	15	15	1
4	69	66	28
5	177	171	32
6	54	57	-37
7	132	137	-40
8	31	36	-84
9	70	72	-22
10	-2	14	-59
11	62	66	-41
12	72	71	4
13	26	25	1
14	50	50	0
15	51	50	10

-4 3 1

1	46	44	18
2	104	105	-13
3	125	127	-9
4	86	83	29
5	105	103	15
6	195	190	26
7	111	110	14
8	83	69	106
9	113	115	-10
10	92	88	25
11	110	110	5
12	47	45	23
13	61	64	-30
14	34	31	35
15	16	16	0
16	34	27	87

-3 3 1

1	242	238	14
2	103	100	25
3	61	62	-8
4	151	154	-21
5	155	158	-18
6	117	117	2
7	78	78	-3
8	42	46	-43
9	56	55	12
10	93	94	-6
11	183	181	12
12	106	105	7
13	64	66	-26
14	63	64	-12
15	72	69	26
16	33	34	-1

-2 3 1

1	103	99	34
2	137	146	-66
3	74	71	27
4	31	31	-1
5	152	154	-14
6	162	161	9
7	106	101	38
8	105	110	-41
9	112	112	0
10	110	105	37
11	141	143	-15
12	119	120	-7
13	77	77	-1
14	56	57	-6
15	8	7	2
16	28	27	24
17	34	35	-15

-1 3 1

1	55	62	-93
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3	162	169	-47
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5	83	84	-6
6	123	128	-39
7	89	91	-22
8	112	113	-8
9	53	53	0
10	120	121	-10
11	199	198	6
12	49	48	5
13	83	86	-18
14	46	45	13
15	38	38	10
16	24	26	-19
17	32	28	54

0 3 1

1	132	125	61
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3	203	201	13
4	63	64	-16
5	96	98	-29
6	46	51	-82
7	38	34	79
8	104	104	0
9	60	61	-10
10	120	115	44
11	126	132	-45
12	106	107	-10
13	55	54	17
14	18	18	2
15	62	64	-24
16	49	48	12
17	22	23	-6

1 3 1

0	229	230	-2
1	46	35	117
2	349	348	3
3	110	113	-24
4	91	85	51
5	132	118	97
6	161	162	-7
7	228	227	4
8	87	85	19
9	23	26	-37
10	49	50	-10
11	206	212	-31
12	153	151	11
13	42	46	-42
14	33	36	-49
15	25	20	64
16	24	27	-35
17	15	17	-11

2 3 1

0	142	135	42
1	40	46	-96
2	244	235	40
3	54	61	-75
4	148	149	-9
5	123	122	6
6	102	101	11
7	104	105	-11
8	113	122	-65
9	112	109	27
10	50	55	-65
11	118	120	-17
12	21	24	-43
13	37	32	58
14	35	37	-16
15	72	72	-1
16	52	52	7
17	-12	7	-19

3 3 1

0	117	118	-11
1	56	59	-31
2	63	62	11
3	210	210	0
4	39	40	-11
5	59	64	-49
6	70	67	27
7	54	52	20
8	88	89	-11
9	52	56	-51
10	123	120	20
11	83	79	32
12	45	47	-31
13	57	53	38
14	23	25	-26
15	23	24	-16
16	31	29	23

4 3 1

0	210	204	29
1	166	166	4
2	169	152	95
3	184	182	14
4	139	132	47
5	244	246	-9
6	83	88	-49
7	280	270	38
8	103	105	-11
9	63	60	34
10	48	48	-7
11	77	78	-14
12	26	25	15
13	15	17	-26
14	43	43	10
15	49	49	4

5 3 1

0	41	42	-10
1	28	29	-14
2	96	96	0
3	109	109	0
4	59	56	35
5	126	124	14
6	30	27	51
7	54	50	55
8	102	99	27
9	128	129	-11
10	56	56	9
11	23	23	2
12	48	47	17
13	51	51	10
14	19	24	-54
15	41	39	28

6 3 1

0	96	94	14
1	112	104	57
2	43	39	47
3	86	85	4
4	113	115	-15
5	191	198	-35
6	206	204	8
7	131	130	4
8	33	29	65
9	46	48	-20
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11	45	47	-23
12	21	25	-54
13	23	19	50

7 3 1

0	22	26	-47
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2	76	70	46
3	32	30	32
4	67	65	16
5	79	74	34
6	139	142	-14
7	58	53	50
8	66	64	21
9	40	42	-28
10	40	42	-30
11	-7	7	-33
12	27	28	-5

8 3 1

0	45	46	-19
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2	-8	9	-41
3	60	56	36
4	36	36	1
5	88	85	22
6	84	81	17
7	49	47	22
8	12	12	1
9	43	42	21
10	22	23	-13

9 3 1

0	42	42	5
1	40	36	54
2	27	23	49
3	20	19	10
4	27	24	42
5	145	141	31
6	40	38	25
7	68	67	15
8	29	25	43

10 3 1

0	21	23	-19
1	15	20	-47
2	44	43	12
3	21	22	-8
4	-4	5	-13

-9 4 1

1	19	18	3
2	8	13	-20
3	25	25	0
4	15	21	-72
5	26	21	55
6	13	15	-14

-8 4 1

1	30	29	18
2	6	8	-10
3	68	67	11
4	39	43	-59
5	62	62	6
6	49	43	76
7	28	25	31
8	19	18	8
9	11	13	-16

-7 4 1

1	26	26	-7
2	25	25	5
3	23	23	0

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4	45	49	-59
5	58	53	46
6	48	44	51
7	94	92	15
8	33	36	-43
9	23	26	-42
10	25	25	0
11	27	32	-68

-6 4 1

1	53	47	56
2	68	66	22
3	68	70	-24
4	70	74	-41
5	97	94	21
6	77	72	38
7	21	19	20
8	81	83	-11
9	25	23	27
10	22	24	-32
11	31	32	-27
12	-13	6	-49
13	21	23	-17

-5 4 1

1	47	45	26
2	33	32	26
3	53	48	49
4	59	57	16
5	32	30	34
6	113	111	14
7	127	130	-20
8	17	17	3
9	70	72	-18
10	62	62	-8
11	52	55	-40
12	13	17	-40
13	39	42	-34
14	39	39	9

-4 4 1

1	61	59	15
2	112	107	37
3	3	12	-47
4	68	62	53
5	119	116	22
6	71	68	25
7	178	176	11
8	82	79	20
9	25	22	37
10	46	43	34
11	90	92	-8
12	35	36	-17
13	33	35	-32
14	44	40	61

-3 4 1

1	30	27	21
2	79	79	0
3	83	82	3
4	60	62	-19
5	101	98	30
6	166	165	5
7	207	207	1
8	141	147	-35
9	112	113	-8
10	85	84	14
11	77	78	-13
12	28	29	-16
13	48	51	-40
14	39	41	-38
15	10	11	-5

-2 4 1

1	89	91	-18
2	162	155	44
3	76	70	46
4	48	48	5
5	147	146	5
6	124	124	0
7	229	228	4
8	122	121	2
9	49	47	25
10	97	99	-16
11	60	63	-22
12	40	40	-9
13	22	22	-9
14	49	48	13
15	54	54	-5

-1 4 1

1	86	90	-37
2	112	117	-39
3	54	51	31
4	68	70	-19
5	121	12[illegible]	4
6	231	[illegible]3	-9
7	63	64	-10
8	103	109	-51
9	52	50	18
10	67	65	14
11	19	20	-14
12	19	20	-5
13	46	45	4
14	3	11	-32
15	64	65	-17
16	36	38	-23

0 4 1

0	95	77	140
1	223	221	13
2	104	95	87
3	125	124	13
4	73	75	-24
5	81	83	-13
6	169	167	11
7	106	106	7
8	31	35	-95
9	-4	7	-33
10	34	35	-27
11	51	48	45
12	72	71	7
13	15	19	-47
14	33	31	21
15	60	61	-14
16	31	34	-44

1 4 1

0	7	3	13
1	25	26	-8
2	82	88	-57
3	37	37	12
4	70	70	-1
5	176	181	-24
6	77	77	6
7	124	126	-10
8	72	72	0
9	55	52	32
10	40	44	-52
11	49	51	-20
12	56	57	-9
13	44	43	19
14	40	43	-47
15	96	104	-72
16	32	34	-38

2 4 1

0	67	64	24
1	137	128	59
2	102	100	14
3	79	76	29
4	80	82	-20
5	12	15	-16
6	187	185	13
7	96	95	8
8	15	16	-9
9	23	25	-23
10	20	18	17
11	84	81	21
12	39	40	-20
13	35	35	-9
14	44	46	-38
15	40	39	16

3 4 1

0	42	45	-28
1	130	129	5
2	132	124	52
3	126	129	-26
4	169	163	31
5	186	184	6
6	26	22	62
7	182	182	-1
8	52	48	40
9	82	82	2
10	32	36	-64
11	84	80	28
12	75	76	-7
13	46	44	19
14	74	72	23
15	51	52	-15

4 4 1

0	89	86	19
1	101	100	11
2	36	34	43
3	123	119	27
4	72	71	9
5	139	141	-14
6	174	172	12
7	44	47	-37
8	25	26	-17
9	58	59	-13
10	16	18	-10
11	32	34	-26
12	49	47	30
13	50	50	-5
14	29	29	5

5 4 1

0	76	75	9
1	238	234	15
2	145	152	-48
3	165	165	4
4	118	120	-14
5	172	170	10
6	123	119	25
7	88	92	-26
8	28	34	-79
9	47	50	-33
10	38	38	13
11	35	40	-69
12	36	39	-46
13	17	15	13

6 4 1

0	40	40	4
1	97	101	-31
2	87	84	23
3	87	87	-3
4	71	69	17
5	89	92	-27
6	82	80	17
7	33	31	30
8	28	30	-23
9	51	56	-57
10	47	50	-42
11	10	10	2
12	46	44	26

7 4 1

0	84	79	36
1	100	93	45
2	65	65	-1
3	61	63	-18
4	77	76	8
5	40	38	21
6	58	62	-53
7	-4	8	-34
8	31	31	-2
9	40	35	65
10	34	35	-17

8 4 1

0	27	31	-56
1	48	42	73
2	29	27	23
3	14	16	-12
4	33	33	-1
5	64	61	28
6	20	21	-6
7	-6	12	-37
8	20	20	-5

9 4 1

0	32	29	40
1	18	22	-41
2	37	37	10
3	35	32	45
4	33	31	30
5	44	42	32

-8 5 1

1	55	57	-27
2	10	16	-42
3	26	27	-16
4	25	24	8
5	23	23	9
6	11	15	-4

-7 5 1

1	54	58	-47
2	21	23	-23
3	17	17	0
4	42	40	26
5	39	40	-3
6	50	45	59
7	14	14	0
8	42	45	-37

-6 5 1

1	84	85	-2
2	64	59	40
3	102	100	16
4	60	59	11
5	47	43	58
6	39	41	-35
7	68	65	32
8	-6	10	-44
9	18	22	-55
10	38	35	44

-5 5 1

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1	127	128	-9
2	59	59	0
3	81	83	-15
4	16	17	-8
5	30	33	-52
6	64	61	28
7	47	48	-13
8	53	57	-53
9	52	55	-33
10	30	32	-18
11	31	31	3
12	10	15	-27

-4 5 1

1	94	89	32
2	113	112	4
3	185	180	25
4	149	145	27
5	135	131	28
6	108	105	20
7	40	40	-3
8	52	51	2
9	44	47	-41
10	36	41	-82
11	31	36	-80
12	39	35	51
13	50	48	7

-3 5 1

1	126	120	44
2	37	39	-39
3	117	118	-12
4	80	80	0
5	38	34	56
6	50	49	18
7	162	160	11
8	47	51	-50
9	17	20	-30
10	38	38	0
11	45	44	10
12	36	39	-48
13	23	23	0

-2 5 1

1	58	52	62
2	119	111	56
3	184	180	23
4	147	145	12
5	162	159	17
6	106	100	40
7	85	83	17
8	48	53	-62
9	58	61	-20
10	47	49	-24
11	-8	8	-24
12	42	41	19
13	17	20	-33
14	48	49	-9

-1 5 1

1	101	98	21
2	88	82	43
3	112	105	46
4	25	21	50
5	136	138	-8
6	87	89	-20
7	134	135	-5
8	64	62	22
9	12	15	-20
10	34	34	1
11	44	43	11
12	29	30	-25
13	31	31	4
14	38	37	10

0 5 1

1	91	90	0
2	55	55	8
3	49	49	2
4	48	45	44
5	144	137	50
6	46	41	69
7	133	130	26
8	82	79	30
9	36	33	50
10	13	20	-84
11	32	34	-40
12	32	32	-17
13	31	32	-19
14	7	15	-87

1 5 1

0	69	69	2
1	61	60	5
2	61	54	69
3	109	102	48
4	96	93	19
5	83	85	-12
6	158	157	3
7	74	70	36
8	80	82	-10
9	52	56	-54
10	45	40	57
11	19	19	-6
12	14	19	-57
13	32	30	26
14	35	36	-14

2 5 1

0	68	63	37
1	88	87	7
2	69	64	40
3	17	17	3
4	81	77	36
5	122	118	21
6	-8	4	-17
7	130	130	1
8	70	65	43
9	23	20	38
10	28	33	-81
11	66	67	-7
12	46	46	12
13	34	33	23

3 5 1

0	87	84	23
1	54	55	-9
2	99	100	-2
3	64	57	61
4	110	110	0
5	60	60	0
6	87	84	22
7	107	108	-11
8	43	47	-54
9	61	59	9
10	27	29	-25
11	42	43	-19
12	43	42	9
13	37	32	70

4 5 1

0	69	66	27
1	102	99	23
2	116	117	-6
3	70	74	-36
4	72	72	0
5	88	86	12
6	38	40	-23
7	72	70	12
8	60	57	25
9	50	50	-11
10	55	53	27
11	59	58	15
12	50	48	30

5 5 1

0	55	56	-2
1	73	79	-57
2	52	58	-71
3	43	44	-17
4	28	28	5
5	78	83	-39
6	61	66	-49
7	17	22	-53
8	62	60	17
9	20	19	10
10	45	49	-61
11	19	24	-44

6 5 1

0	60	60	-1
1	70	65	45
2	37	33	50
3	42	44	-31
4	51	53	-26
5	25	27	-17
6	22	26	-52
7	44	46	-30
8	45	47	-39
9	-6	1	-15
10	46	43	34

7 5 1

0	24	24	0
1	56	57	-13
2	54	52	18
3	24	23	22
4	9	18	-89
5	50	50	-3
6	36	36	-2
7	14	16	-19
8	23	25	-25

8 5 1

0	17	17	0
1	31	30	1
2	42	44	-32
3	7	11	-22
4	21	20	13
5	2	16	-47

-7 6 1

1	18	23	-50
2	11	13	-6
3	29	28	0

-6 6 1

1	30	30	-1
2	22	27	-69
3	30	29	18
4	33	34	-20
5	52	52	-6
6	21	20	4

-5 6 1

1	35	33	25
2	89	92	-20
3	61	63	-22
4	52	50	33
5	30	28	88
6	115	113	15
7	48	47	8
8	39	37	34

-4 6 1

1	58	55	36
2	38	34	53
3	32	28	56
4	93	95	-19
5	27	29	-22
6	66	68	-18
7	16	14	12
8	34	36	-21
9	43	44	-16
10	16	18	-9

-3 6 1

1	77	73	25
2	110	112	-13
3	65	61	31
4	94	85	64
5	33	36	-41
6	59	61	-19
7	45	46	-1
8	-8	5	-35
9	42	42	-5
10	40	39	5

-2 6 1

1	62	59	25
2	11	12	-5
3	75	74	3
4	80	77	23
5	19	19	3
6	19	24	-53
7	11	15	-23
8	61	63	-16
9	47	45	20
10	-5	4	-11
11	41	39	36

-1 6 1

1	99	99	0
2	78	77	10
3	47	47	2
4	28	27	12
5	41	42	-13
6	6	13	-35
7	30	30	3
8	41	40	17
9	73	71	12
10	14	17	-25
11	29	32	-48

0 6 1

0	90	90	-2
1	42	43	-15
2	27	27	10
3	58	54	57
4	74	70	43
5	33	34	-26
6	29	31	-45
7	56	47	110
8	39	39	1
9	33	32	10
10	23	25	-26
11	38	37	28

1 6 1

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0	56	53	37
1	129	127	13
2	78	72	45
3	20	21	-11
4	90	91	-4
5	25	31	-91
6	38	38	8
7	11	17	-43
8	85	86	-10
9	51	48	39
10	-4	15	-81
11	48	48	0

2 6 1

0	37	39	-28
1	104	106	-14
2	8	6	4
3	91	87	29
4	52	51	1
5	35	35	-1
6	37	37	-1
7	63	55	72
8	15	19	-51
9	29	26	41
10	30	28	17
11	24	21	26

3 6 1

0	162	159	18
1	137	129	47
2	21	17	40
3	31	34	-43
4	39	42	-43
5	37	34	40
6	66	65	6
7	46	46	-6
8	62	63	-6
9	21	20	14
10	34	35	-18

4 6 1

0	81	83	-16
1	27	24	44
2	31	31	-4
3	53	53	2
4	20	18	18
5	-7	7	-18
6	53	55	-28
7	50	52	-27
8	12	15	-14
9	32	31	16

5 6 1

0	104	102	14
1	31	31	0
2	-4	7	-10
3	19	21	-25
4	35	34	17
5	47	44	39
6	-6	8	-31
7	61	59	19
8	38	41	-46

6 6 1

0	17	18	-18
1	39	39	-2
2	25	27	-27
3	22	22	3
4	9	11	-8
5	27	29	-37
6	50	50	-5

7 6 1

0	20	20	0
1	-8	6	-21
2	15	20	-53

-4 7 1

1	11	11	0
2	29	35	-100
3	26	28	-20
4	14	15	-5

-3 7 1

1	48	48	-8
2	13	17	-38
3	10	19	-78
4	40	43	-42
5	19	20	-11
6	34	32	26

-2 7 1

1	17	20	-34
2	37	40	-34
3	15	16	-12
4	20	18	28
5	14	19	-60
6	48	47	9
7	10	9	3

-1 7 1

1	50	48	19
2	5	15	-67
3	36	38	-36
4	36	39	-51
5	45	43	33
6	3	11	-43
7	43	42	18

0 7 1

1	62	65	-47
2	42	40	40
3	27	28	-23
4	22	23	-11
5	47	48	-20
6	42	40	55
7	-13	2	-68
8	32	29	55

1 7 1

0	107	105	15
1	34	34	-2
2	24	24	5
3	29	25	61
4	24	27	-40
5	51	50	17
6	24	23	6
7	11	13	-10

2 7 1

0	73	74	-5
1	41	41	5
2	52	53	-12
3	22	20	18
4	61	65	-47
5	86	83	23
6	9	13	-18
7	10	13	-16

3 7 1

0	67	68	-14
1	10	14	-31
2	33	33	2
3	34	33	21
4	64	62	20
5	45	43	23
6	-4	11	-36

4 7 1

0	53	51	18
1	36	37	-7
2	28	31	-41
3	38	38	1
4	92	92	-1

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Table S5E. Observed and Calculated Structure Factors for 4′-Bromo-N-methyl-4-stilbazolium Chloride

The columns contain, in order, h, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

I-1147-M58

h	0	-13	
2	249	226	21
4	59	77	-7

h	0	-12	
0	401	391	10
2	322	320	1
4	121	105	11
6	206	219	-12

h	0	-11	
2	524	516	8
4	369	360	9
6	378	350	28
8	236	225	8

h	0	-10	
0	660	656	3
2	224	227	-3
4	694	673	21
6	138	137	1
8	154	148	5
10	500	473	25

h	0	-9	
2	576	570	6
4	244	250	-5
6	424	406	19
8	275	268	6
10	191	192	-1
12	343	280	53

h	0	-8	
0	514	519	-7
2	601	586	19
4	712	697	16
6	248	229	19
8	93	103	-7
10	521	467	56
12	178	156	20

h	0	-7	
2	583	582	1
4	566	543	29
6	522	509	16
8	406	390	20
10	204	199	5
12	231	219	10
14	80	68	4

h	0	-6	
0	947	935	11
2	608	612	-4
4	1237	1200	27
6	375	366	12
8	494	469	31
10	452	423	33
12	394	346	48
14	200	183	16

h	0	-5	
2	1272	1254	13
4	808	767	44
6	814	772	43
8	699	662	41
10	166	156	12
12	369	334	36
14	359	356	2

h	0	-4	
0	969	962	6
2	156	156	0
4	755	734	25
6	714	690	28
8	849	804	44
10	590	547	49
12	135	142	-6
14	373	360	11
16	116	77	20

h	0	-3	
2	1018	988	27
4	845	814	33
6	664	634	37
8	504	476	37
10	318	294	28
12	461	440	22
14	104	104	0
16	191	160	27

h	0	-2	
0	419	411	15
2	575	559	24
4	637	620	23
6	888	847	41
8	817	789	29
10	264	258	7
12	180	174	8
14	456	416	39
16	63	18	10

h	0	-1	
2	1131	1117	12
4	1387	1358	20
6	1487	1435	33
8	746	721	27
10	432	394	48
12	293	288	5
14	47	29	4
16	295	264	24

h	0	0	
2	859	891	-37
4	127	119	12
6	581	578	3
8	853	826	28
10	1004	920	72
12	150	100	45
14	496	440	57
16	87	79	4

h	0	1	
2	1116	1187	-64
4	1368	1416	-35
6	1531	1529	1
8	778	759	21
10	382	371	13
12	254	266	-12
14	50	29	3
16	295	256	42

h	0	2	
0	569	571	-3
2	561	589	-47
4	652	677	-36
6	777	799	-25
8	740	748	-8
10	346	328	22
12	181	195	-13
14	437	413	25
16	80	25	15

h	0	3	
2	916	962	-49
4	796	834	-45
6	622	632	-14
8	467	465	2
10	303	305	-3
12	444	442	2
14	88	107	-12
16	174	157	16

h	0	4	
0	999	1004	-4
2	141	146	-7
4	739	774	-43
6	615	640	-33
8	735	739	-4
10	621	615	6
12	142	131	11
14	348	323	24
16	105	82	9

h	0	5	
2	1228	1217	12
4	782	792	-12
6	767	784	-20
8	633	646	-16
10	141	149	-9
12	353	339	14
14	364	353	14

h	0	6	
0	776	783	-7
2	593	619	-35
4	1224	1267	-34
6	311	319	-11
8	479	494	-19
10	407	413	-6
12	358	363	-6
14	214	207	7

h	0	7	
2	585	598	-17
4	501	513	-16
6	455	489	-47
8	379	379	-1
10	226	230	-3
12	256	245	12
14	96	71	13

h	0	8	
0	528	525	3
2	586	590	-6
4	650	675	-29
6	239	243	-3
8	53	67	-4
10	458	467	-10
12	159	147	12

h	0	9	
2	561	580	-23
4	210	217	-6
6	375	378	-4
8	272	277	-5
10	169	169	0
12	271	265	6

h	0	10	
0	636	638	-1
2	218	224	-5
4	636	652	-17
6	168	175	-7
8	174	177	-3
10	462	456	7

h	0	11	
2	534	551	-19
4	372	377	-6
6	352	353	-1
8	244	232	14

h	0	12	
0	423	433	-15
2	302	308	-7
4	129	118	9
6	259	265	-7

h	0	13	
2	205	197	10
4	38	52	-3

h	1	-13	
0	371	374	-4
1	-5	12	0
2	131	118	13
3	67	52	6

h	1	-12	
1	-20	25	-3
2	310	303	9
3	36	43	-2
4	126	135	-10
5	-42	69	-22
6	293	293	0
7	41	51	-3

h	1	-11	
0	107	106	1
1	139	137	2
2	397	387	14
3	65	66	0
4	418	401	23
5	50	22	9
6	354	330	30
7	68	32	13
8	204	182	30
9	50	24	4

h	1	-10	
1	90	84	5
2	489	486	4
3	147	134	18
4	232	227	6
5	61	31	8
6	340	319	30
7	-63	44	-22
8	261	259	3
9	55	42	4
10	181	174	8
11	-25	22	-1

h	1	-9	
0	992	988	4
1	44	32	3
2	118	108	14
3	97	91	6
4	258	246	18
5	41	20	6

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6	484	474	15
7	109	100	0
8	353	330	31
9	13	52	-9
10	136	127	10
11	38	17	4
12	82	59	12

h 1 -8

1	28	36	-2
2	506	500	9
3	-20	31	-6
4	135	129	8
5	63	61	0
6	381	371	16
7	-31	23	-5
8	337	324	19
9	29	55	-9
10	195	177	24
11	-51	17	-8
12	162	152	11
13	-67	22	-12

h 1 -7

0	1049	1049	0
1	52	50	1
2	51	44	4
3	52	59	-4
4	426	415	20
5	68	33	22
6	607	590	25
7	178	183	-8
8	653	630	32
9	41	32	3
10	289	269	26
11	38	38	0
12	241	230	12
13	-57	16	-9
14	249	238	12

h 1 -6

1	217	212	9
2	1259	1200	51
3	186	174	22
4	694	660	48
5	65	54	10
6	101	115	-22
7	46	60	-6
8	255	248	11
9	-35	42	-11
10	352	344	12
11	47	23	5
12	436	419	23
13	63	49	5
14	166	162	4

h 1 -5

0	980	982	-2
1	310	301	18
2	490	479	19
3	111	112	-2
4	627	612	22
5	81	77	5
6	659	643	24
7	44	73	-14
8	498	468	47
9	-58	24	-15
10	458	442	26
11	50	49	0
12	92	75	14
13	-80	32	-20
14	435	418	21
15	-72	31	-14

h 1 -4

1	122	124	-5
2	1226	1200	23
3	32	29	1
4	186	184	3
5	196	197	-2
6	674	653	31
7	108	107	1
8	595	567	43
9	-37	89	-37
10	440	421	29
11	50	61	-3
12	598	574	33
13	36	31	1
14	128	121	6
15	60	17	8

h 1 -3

0	885	887	-2
1	63	63	0
2	743	722	30
3	150	146	9
4	1418	1367	40
5	36	23	4
6	396	380	32
7	124	120	6
8	400	373	48
9	-38	42	-13
10	595	566	42
11	102	100	2
12	267	269	-2
13	19	37	-3
14	292	282	12
15	-39	24	-5
16	240	227	14

h 1 -2

1	74	70	9
2	957	939	21
3	76	67	18
4	791	767	33
5	141	140	2
6	761	736	34
7	-29	43	-15
8	406	395	19
9	108	111	-4
10	183	183	0
11	30	59	-8
12	392	380	17
13	-59	42	-16
14	95	87	7
15	-49	15	-6
16	216	196	24

h 1 -1

0	390	394	-12
1	60	61	-2
2	157	142	36
3	181	183	-3
4	1809	1786	15
5	203	195	16
6	342	334	16
7	20	41	-7
8	141	120	42
9	59	68	-8
10	650	641	13
11	-22	72	-20
12	319	319	0
13	-108	16	-34
14	174	168	9
15	-39	34	-7
16	34	41	-1

h 1 0

1	122	118	9
2	786	782	4
3	58	52	10
4	344	343	2
5	65	67	-4
6	720	722	-3
7	-69	31	-31
8	490	486	6
10	169	167	2
12	376	390	-22
13	-120	49	-48
14	105	82	21
16	186	161	34

h 1 1

0	444	442	5
1	59	60	-3
2	147	150	-7
3	171	177	-13
4	1682	1756	-51
5	193	192	2
6	349	341	17
7	58	58	0
8	195	193	4
9	71	67	4
10	620	624	-6
11	31	68	-13
12	303	315	-18
13	-46	18	-7
14	192	192	0
15	-30	35	-9
16	71	36	14

h 1 2

1	57	65	-16
2	896	939	-54
3	65	56	17
4	766	792	-38
5	137	142	-11
6	723	743	-29
7	36	41	-3
8	405	402	6
9	118	118	0
10	189	184	8
11	31	55	-10
12	338	340	-3
13	34	41	-2
14	82	89	-5
15	-32	14	-4
16	230	214	19

h 1 3

0	1018	1018	0
1	66	62	7
2	673	694	-33
3	130	138	-17
4	1256	1288	-29
5	-34	28	-13
6	384	395	-24
7	100	112	-22
8	394	383	21
9	-12	41	-8
10	534	541	-12
11	89	91	-2
12	258	252	8
13	-38	41	-9
14	267	265	1
15	15	29	-2
16	233	221	18

h 1 4

1	122	126	-10
2	1147	1196	-49
3	-25	37	-15
4	162	152	20
5	187	195	-16
6	619	644	-40
7	111	107	5
8	569	572	-5
9	27	91	-43
10	428	430	-3
11	20	60	-16
12	568	569	-1
13	-73	29	-18
14	112	118	-5
15	-63	16	-13

h 1 5

0	1010	1013	-3
1	306	312	-13
2	439	449	-21
3	89	96	-12
4	571	595	-43
5	82	73	13
6	658	681	-34
7	41	67	-18
8	487	497	-17
9	22	25	0
10	383	392	-15
11	-33	54	-13
12	81	88	-6
13	40	36	1
14	472	460	19
15	59	34	6

h 1 6

1	203	205	-4
2	1172	1172	0
3	163	168	-10
4	649	652	-5
5	62	70	-9
6	162	163	-2
7	63	61	1
8	252	267	-24
9	42	49	-3
10	331	340	-14
11	54	21	8
12	410	412	-3
13	39	46	-2
14	149	162	-18

h 1 7

0	1071	1085	-14
1	-37	42	-16
2	37	50	-9
3	19	61	-17
4	379	391	-23
5	-12	32	-7
6	573	606	-53
7	184	189	-8
8	635	649	-20
9	8	31	-4
10	295	291	6
11	-52	30	-11
12	207	216	-13
13	-24	16	-2
14	243	228	19

h 1 8

1	48	43	2
2	521	532	-19
3	9	28	-3
4	118	119	0
5	37	66	-17
6	349	353	-6
7	29	23	1
8	318	324	-9

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9	-6	49	-10
10	172	174	-3
11	-38	19	-8
12	180	181	0
13	-30	26	-5

h 1 9

0	968	972	-4
1	53	43	6
2	117	125	-12
3	98	87	10
4	242	246	-5
5	-24	20	-3
6	458	463	-8
7	103	96	6
8	322	320	2
9	79	52	18
10	117	111	6
11	61	22	10
12	56	69	-6

h 1 10

1	100	88	12
2	489	503	-23
3	130	138	-9
4	242	243	0
5	26	20	0
6	326	339	-19
7	64	43	9
8	255	268	-19
9	-43	40	-11
10	146	153	-8
11	-30	24	-3

h 1 11

0	60	84	-16
1	140	130	13
2	402	403	-1
3	84	77	4
4	394	405	-16
5	69	20	19
6	312	313	0
7	84	38	23
8	162	165	-3
9	-69	24	-16

h 1 12

1	-31	23	-5
2	255	272	-24
3	69	41	13
4	106	115	-9
5	51	68	-6
6	290	295	-5
7	58	51	2

h 1 13

0	339	342	-3
1	79	10	20
2	120	117	2
3	41	50	-3

h 2 -12

0	306	306	0
1	52	16	6
2	218	215	3
3	-39	46	-13
4	87	68	9
5	22	16	0

h 2 -11

1	144	143	1
2	495	506	-15
3	69	75	-3
4	171	164	9
5	104	81	18
6	208	202	7
7	-26	4	-1
8	232	213	23

h 2 -10

0	365	361	5
1	82	88	-5
2	352	347	7
3	176	163	19
4	558	541	23
5	98	91	6
6	166	161	6
7	68	92	-13
8	184	196	-17
9	50	54	-1
10	360	328	37

h 2 -9

1	120	113	9
2	453	443	14
3	84	79	4
4	206	201	7
5	126	119	7
6	355	340	20
7	46	55	-3
8	223	209	18
9	56	77	-10
10	118	119	-1
11	-58	29	-10

h 2 -8

0	465	470	-9
1	87	88	-1
2	458	455	4
3	239	239	0
4	625	611	19
5	44	52	-2
6	114	109	5
7	101	85	16
8	115	116	-1
9	-63	32	-20
10	388	362	35
11	23	76	-13
12	101	99	1

h 2 -7

1	47	70	-19
2	546	544	2
3	113	107	8
4	303	300	5
5	131	128	5
6	334	321	20
7	124	96	35
8	453	436	25
9	55	39	4
10	117	133	-18
11	-17	52	-11
12	146	139	7
13	-58	45	-13

h 2 -6

0	659	651	11
1	140	130	17
2	258	250	14
3	187	178	12
4	824	801	28
5	162	157	6
6	313	305	14
7	79	88	-9
8	197	182	20
9	47	24	5
10	495	469	36
11	161	166	-7
12	342	346	-5
13	-40	50	-14
14	176	166	10

h 2 -5

1	118	122	-9
2	311	307	7
3	186	184	3
4	230	238	-14
5	202	194	12
6	1129	1087	40
7	142	135	11
8	421	410	18
9	130	126	4
10	203	199	6
11	-35	11	-5
12	134	150	-18
13	127	109	18
14	229	230	0

h 2 -4

0	1174	1173	1
1	201	204	-5
2	732	718	20
3	194	186	13
4	716	702	20
5	129	119	20
6	344	327	33
7	156	151	7
8	368	349	32
9	165	163	2
10	362	360	3
11	96	97	-1
12	106	114	-8
13	-9	38	-5
14	338	337	0
15	64	64	0

h 2 -3

1	196	192	9
2	942	916	29
3	116	114	2
4	341	330	23
5	191	195	-6
6	360	358	3
7	8	20	-1
8	449	441	14
9	133	142	-14
10	239	239	0
11	-55	27	-17
12	361	372	-16
13	-43	49	-12
14	48	98	-17
15	51	55	-1

h 2 -2

0	795	805	-14
1	201	197	8
2	838	814	31
3	212	204	17
4	344	334	21
5	47	58	-9
6	590	588	2
7	232	218	23
8	516	498	29
9	-25	3	-2
10	238	247	-13
11	55	63	-3
12	117	125	-8
13	25	51	-5
14	326	314	14
15	50	49	0
16	42	44	0

h 2 -1

1	153	159	-11
2	1556	1525	23
3	447	435	23
4	250	242	16
5	356	352	9
6	467	463	6
7	115	112	5
8	708	689	26
9	181	173	15
10	245	261	-24
11	-76	6	-20
12	281	310	-41
13	77	59	10
14	29	49	-4
15	-46	49	-11
16	212	223	-13

h 2 0

0	3178	3088	47
1	577	585	-14
2	1925	1951	-15
3	612	621	-15
4	261	257	6
5	93	85	13
6	858	868	-13
7	288	296	-16
8	1230	1197	29
9	88	102	-16
10	378	375	5
11	94	130	-44
12	194	206	-16
13	120	143	-27
14	338	328	12
15	72	80	-4
16	22	26	0

h 2 1

1	159	160	-2
2	1586	1622	-26
3	443	452	-18
4	202	194	16
5	380	379	3
6	470	475	-9
7	102	109	-11
8	726	744	-26
9	192	186	9
10	222	230	-12
11	-43	11	-9
12	287	322	-50
13	13	63	-11
14	53	51	1
15	-62	44	-18
16	232	209	34

h 2 2

0	778	774	6
1	184	189	-12
2	812	838	-36
3	234	236	-5
4	397	415	-39
5	47	67	-19
6	545	575	-54
7	196	208	-20
8	480	492	-20
9	24	4	2
10	241	261	-30
11	40	80	-17
12	135	141	-8
13	-24	50	-9

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14	290	303	-20
15	74	47	13
16	8	49	-5

h 2 3

1	194	192	3
2	891	921	-47
3	92	97	-11
4	319	330	-22
5	179	198	-35
6	328	343	-30
7	-25	24	-6
8	403	414	-21
9	127	136	-14
10	215	222	-9
11	57	29	8
12	378	390	-17
13	-53	53	-16
14	95	99	-3
15	39	57	-6

h 2 4

0	1069	1071	-1
1	179	187	-16
2	733	747	-20
3	184	195	-21
4	721	749	-40
5	124	127	-5
6	309	324	-31
7	134	139	-8
8	317	322	-8
9	161	165	-5
10	378	393	-24
11	75	89	-10
12	84	100	-14
13	-56	33	-12
14	303	304	-1
15	13	59	-9

h 2 5

1	119	121	-4
2	316	327	-24
3	179	181	-4
4	201	216	-27
5	186	189	-5
6	1047	1075	-30
7	124	134	-16
8	397	403	-10
9	124	126	-2
10	180	189	-15
11	-19	14	-2
12	170	175	-7
13	92	108	-12
14	238	228	13

h 2 6

0	623	617	9
1	132	136	-7
2	214	215	-1
3	182	183	-1
4	809	844	-46
5	171	164	12
6	243	242	1
7	71	77	-5
8	166	163	5
9	-55	21	-12
10	473	483	-15
11	174	176	-3
12	339	361	-37
13	-13	44	-6
14	185	182	3

h 2 7

1	42	69	-13
2	507	522	-25
3	84	97	-15
4	293	300	-12
5	125	137	-20
6	325	346	-37
7	91	99	-7
8	412	416	-7
9	-18	46	-11
10	150	165	-21
11	33	50	-5
12	159	153	7
13	25	47	-5

h 2 8

0	473	474	-1
1	90	86	4
2	460	461	-1
3	230	238	-12
4	582	605	-32
5	49	47	1
6	104	96	9
7	42	77	-14
8	66	66	0
9	-26	33	-5
10	344	365	-33
11	71	73	-1
12	61	87	-15

h 2 9

1	110	107	3
2	409	416	-12
3	92	84	6
4	222	212	14
5	103	106	-3
6	322	336	-20
7	-16	52	-9
8	223	226	-4
9	80	72	4
10	111	113	-2
11	74	29	15

h 2 10

0	386	384	2
1	93	90	2
2	340	339	2
3	161	157	5
4	512	521	-13
5	104	89	14
6	162	168	-8
7	57	94	-27
8	183	195	-18
9	54	54	0
10	310	317	-9

h 2 11

1	152	153	0
2	520	535	-22
3	76	74	0
4	187	179	12
5	90	86	3
6	179	191	-18
7	72	6	21
8	216	223	-8

h 2 12

0	326	326	0
1	-40	24	-7
2	194	207	-19
3	62	49	5
4	109	109	0
5	-16	10	-1

h 3 -12

1	100	98	1

h 3 -11

0	-58	22	-10
1	91	46	23
2	276	272	5
3	34	42	-2
4	267	261	6
5	70	47	9
6	297	268	31

h 3 -10

1	123	115	8
2	334	329	6
3	49	41	2
4	128	125	4
5	148	159	-13
6	180	176	5
7	40	20	3
8	207	194	17

h 3 -9

0	473	471	1
1	195	197	-2
2	92	76	14
3	38	76	-13
4	221	208	16
5	-68	39	-24
6	355	345	13
7	155	145	13
8	257	262	-4
9	-18	59	-15
10	42	30	2

h 3 -8

1	80	90	-8
2	357	355	2
3	92	95	-3
4	209	192	22
5	98	99	-1
6	261	243	22
7	-38	27	-9
8	226	224	2
9	122	120	3
10	141	118	24
11	36	8	4

h 3 -7

0	961	957	3
1	280	274	9
2	154	153	1
3	112	86	31
4	223	224	0
5	25	24	0
6	293	282	16
7	237	226	13
8	295	286	11
9	-19	53	-12
10	252	243	9
11	-41	73	-18
12	142	154	-13

h 3 -6

1	243	250	-11
2	634	623	17
3	53	57	-2
4	541	528	21
5	243	234	12
6	121	113	11
7	14	41	-5
8	197	191	8
9	116	110	5
10	293	293	0
11	-74	23	-22
12	216	246	-40
13	54	75	-10

h 3 -5

0	655	654	1
1	175	170	12
2	415	405	18
3	169	160	17
4	454	446	14
5	155	149	9
6	412	388	38
7	215	221	-9
8	282	269	18
9	115	117	-2
10	285	290	-5
11	31	69	-10
12	77	72	2
13	26	74	-11

h 3 -4

1	271	266	9
2	452	441	21
3	83	86	-4
4	436	421	26
5	203	197	10
6	640	617	34
7	66	61	2
8	267	253	21
9	277	268	12
10	288	286	2
11	20	86	-20
12	332	354	-28
13	-8	55	-7
14	115	130	-13

h 3 -3

0	650	654	-7
1	153	153	-1
2	147	141	12
3	354	348	11
4	704	692	17
5	211	197	22
6	296	284	20
7	173	160	18
8	295	295	0
9	109	124	-18
10	476	492	-25
11	150	168	-25
12	201	223	-25
13	27	30	0
14	163	189	-29

h 3 -2

1	239	229	19
2	905	890	18
3	174	171	4
4	271	256	28
5	201	195	8
6	349	340	16
7	33	22	2
8	345	340	8
9	101	97	3
10	101	111	-10
11	-20	39	-6
12	236	263	-34
13	97	117	-14
14	88	105	-12
15	-22	36	-3

h 3 -1

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0	284	283	1
1	90	92	-4
2	404	405	-1
3	334	333	0
4	1113	1092	19
5	202	197	7
6	387	387	0
7	135	144	-18
8	110	112	-3
9	73	82	-6
10	292	314	-33
11	150	172	-32
12	173	186	-17
13	-17	34	-4
14	51	83	-11
15	-88	35	-14

h 3 0

1	197	201	-6
2	548	539	16
3	65	58	7
4	204	199	9
5	208	213	-7
6	476	484	-13
7	85	83	1
8	257	265	-13
9	142	142	0
10	49	50	0
11	-32	60	-20
12	252	288	-50
13	60	76	-9
14	88	69	11
15	71	26	13

h 3 1

0	398	393	11
1	120	120	1
2	386	395	-18
3	319	326	-15
4	1056	1066	-10
5	205	193	19
6	378	385	-12
7	129	138	-15
8	130	145	-23
9	67	81	-13
10	282	308	-39
11	158	172	-19
12	162	185	-34
13	-17	38	-7
14	72	97	-13
15	49	39	3

h 3 2

1	232	234	-4
2	920	926	-6
3	184	175	18
4	208	206	3
5	171	177	-9
6	265	276	-19
7	7	18	-1
8	344	355	-18
9	43	89	-35
10	91	89	1
11	31	34	0
12	192	251	-86
13	90	118	-27
14	84	107	-16
15	46	40	1

h 3 3

0	621	617	5
1	164	156	13
2	182	171	19
3	317	327	-18
4	623	654	-50
5	172	188	-28
6	332	333	0
7	171	174	-5
8	333	341	-12
9	112	122	-13
10	415	458	-71
11	141	156	-20
12	172	212	-55
13	44	31	3
14	173	173	0

h 3 4

1	255	265	-20
2	441	441	0
3	89	86	4
4	390	415	-48
5	187	195	-12
6	598	614	-25
7	63	62	0
8	248	249	-1
9	262	270	-11
10	280	289	-12
11	91	85	4
12	305	355	-82
13	-43	45	-12
14	111	129	-17

h 3 5

0	691	680	15
1	179	182	-5
2	382	383	-2
3	154	160	-10
4	416	417	-2
5	139	138	1
6	420	420	0
7	224	229	-6
8	277	292	-22
9	104	115	-12
10	243	261	-22
11	49	75	-9
12	86	85	1
13	57	81	-9

h 3 6

1	245	246	-1
2	604	619	-23
3	72	75	-3
4	506	515	-15
5	214	223	-14
6	103	111	-8
7	-22	41	-8
8	207	207	0
9	113	113	0
10	277	289	-15
11	13	27	-2
12	214	242	-41
13	52	71	-7

h 3 7

0	992	985	7
1	280	280	1
2	149	147	3
3	66	71	-3
4	211	199	17
5	37	28	2
6	284	285	0
7	235	239	-4
8	288	297	-12
9	54	53	0
10	248	263	-23
11	66	58	3
12	131	145	-14

h 3 8

1	108	100	10
2	327	333	-10
3	92	89	3
4	224	224	0
5	95	111	-17
6	258	269	-14
7	47	25	5
8	219	213	7
9	103	117	-15
10	102	122	-21
11	-64	2	-16

h 3 9

0	461	469	-12
1	190	191	-2
2	70	77	-4
3	82	83	0
4	209	207	3
5	49	43	1
6	333	336	-4
7	118	136	-21
8	244	250	-8
9	37	59	-6
10	68	26	12

h 3 10

1	109	103	5
2	341	343	-2
3	74	51	15
4	128	136	-10
5	175	174	2
6	177	180	-4
7	33	17	3
8	220	208	17

h 3 11

0	18	65	-13
1	84	47	24
2	264	282	-27
3	83	61	12
4	252	266	-20
5	27	50	-5
6	247	254	-10

h 3 12

1	90	97	-6

h 4 -10

0	232	240	-9
1	-30	61	-16
2	168	167	0
3	222	219	4
4	273	274	-2
5	108	108	0

h 4 -9

1	142	136	7
2	231	225	8
3	77	76	0
4	122	105	16
5	152	144	9
6	178	176	1
7	29	37	-1

h 4 -8

0	238	236	3
1	84	99	-13
2	247	245	3
3	191	177	20
4	333	311	29
5	88	82	4
6	88	84	2
7	39	39	0
8	63	46	6
9	92	103	-6

h 4 -7

1	20	87	-23
2	313	305	11
3	74	76	-1
4	189	185	7
5	212	218	-7
6	221	202	25
7	71	48	10
8	236	219	20
9	-30	41	-6
10	91	106	-12

h 4 -6

0	351	352	0
1	70	80	-7
2	128	129	-1
3	272	261	15
4	436	421	24
5	193	190	4
6	155	151	5
7	83	105	-17
8	124	131	-8
9	-25	44	-7
10	222	219	3
11	164	174	-12

h 4 -5

1	110	101	11
2	286	276	17
3	168	160	13
4	87	88	0
5	224	206	22
6	423	427	-6
7	130	113	20
8	270	267	4
9	183	186	-3
10	-44	50	-12
11	-80	34	-19
12	112	94	14

h 4 -4

0	385	384	2
1	282	281	1
2	196	183	19
3	209	205	5
4	344	332	19
5	79	78	0
6	268	246	31
7	166	165	0
8	251	251	0
9	146	160	-19
10	198	209	-15
11	112	118	-4
12	26	60	-6

h 4 -3

1	245	238	11
2	421	403	31
3	112	103	13
4	216	202	20
5	120	118	3
6	226	222	5
7	-55	25	-12
8	203	217	-18
9	140	132	9

10	86	107	-15
11	34	58	-8
12	187	196	-11
13	-33	67	-13

h 4 -2

0	360	362	-2
1	125	121	6
2	213	213	0
3	130	137	-11
4	224	218	8
5	37	63	-13
6	278	276	1
7	240	240	0
8	317	306	15
9	6	33	-3
10	114	121	-6
11	91	81	8
12	34	68	-8
13	88	76	6

h 4 -1

1	187	177	15
2	525	498	44
3	356	345	18
4	324	304	33
5	423	401	35
6	308	304	6
7	75	60	9
8	297	301	-6
9	166	165	1
10	150	155	-7
11	85	50	17
12	126	139	-14
13	63	74	-4

h 4 0

0	1808	1704	63
1	568	544	37
2	503	492	18
3	448	442	10
4	44	49	-1
5	172	192	-35
6	298	298	0
7	361	370	-13
8	424	432	-13
9	94	112	-14
10	265	296	-45
11	137	175	-47
12	92	122	-28
13	124	133	-8

h 4 1

1	184	177	10
2	536	535	0
3	363	365	-3
4	328	330	-4
5	435	434	0
6	333	330	5
7	65	56	4
8	310	324	-22
9	159	166	-12
10	128	140	-14
11	23	57	-8
12	116	138	-25
13	50	79	-17

h 4 2

0	374	367	13
1	118	128	-16
2	234	228	9
3	175	179	-6
4	257	255	3
5	97	74	26
6	268	261	10
7	228	226	3
8	276	291	-22
9	31	35	0
10	129	140	-13
11	103	106	-2
12	38	77	-20
13	35	73	-15

h 4 3

1	242	237	6
2	394	393	2
3	97	89	10
4	215	209	7
5	118	106	17
6	212	221	-13
7	25	25	0
8	203	207	-5
9	123	122	1
10	95	107	-11
11	40	60	-8
12	174	200	-40
13	89	72	10

h 4 4

0	375	370	8
1	253	257	-6
2	212	198	20
3	218	220	-1
4	346	354	-14
5	82	86	-4
6	219	228	-11
7	164	168	-8
8	225	227	-3
9	153	163	-14
10	203	238	-51
11	91	106	-14
12	-28	52	-10

h 4 5

1	106	103	3
2	260	269	-12
3	148	157	-16
4	95	98	-3
5	208	202	9
6	407	426	-31
7	116	113	3
8	259	263	-5
9	177	183	-7
10	-46	41	-13
11	10	41	-6
12	73	103	-22

h 4 6

0	287	288	-1
1	80	58	18
2	127	121	8
3	266	270	-5
4	432	446	-23
5	207	199	11
6	122	121	0
7	93	92	0
8	130	133	-3
9	-43	40	-15
10	201	222	-32
11	169	186	-23

h 4 7

1	112	107	5
2	293	299	-7
3	74	89	-13
4	163	175	-18
5	208	203	6
6	207	202	8
7	29	51	-6
8	189	208	-27
9	-35	60	-19
10	106	120	-14

h 4 8

0	238	239	-3
1	109	93	16
2	245	248	-3
3	182	176	9
4	305	306	-1
5	92	76	13
6	89	91	0
7	-11	11	0
8	-39	19	-6
9	90	103	-11

h 4 9

1	128	120	10
2	216	223	-10
3	-50	63	-22
4	96	101	-4
5	133	147	-17
6	166	170	-5
7	53	36	6

h 4 10

0	228	245	-25
1	77	71	3
2	153	164	-14
3	190	213	-31
4	249	262	-18
5	74	105	-21

h 5 -9

0	301	306	-5
1	155	153	1
2	69	65	1

h 5 -8

1	66	78	-6
2	154	153	1
3	77	72	2
4	94	93	0
5	77	68	4

h 5 -7

0	263	245	20
1	182	164	22
2	86	89	-2
3	97	78	14
4	115	110	4
5	43	11	4
6	195	180	20
7	236	219	21

h 5 -6

1	210	203	9
2	334	327	10
3	54	54	0
4	172	156	23
5	155	149	7
6	-42	27	-7
7	-68	39	-16
8	44	44	0

h 5 -5

0	265	259	8
1	166	160	7
2	140	135	6
3	132	126	8
4	162	157	6
5	121	107	14
6	187	174	19
7	188	171	20
8	151	139	14
9	100	108	-6

h 5 -4

1	242	209	45
2	307	310	-3
3	87	87	0
4	37	46	-2
5	145	130	19
6	91	99	-6
7	68	55	5
8	142	144	-2
9	208	208	0
10	144	148	-4

h 5 -3

0	319	316	5
1	125	124	1
2	253	248	6
3	272	271	2
4	329	323	9
5	121	122	0
6	107	97	9
7	149	136	16
8	124	136	-13
9	66	78	-7
10	148	143	5
11	-43	133	-50

h 5 -2

1	157	149	14
2	229	200	39
3	44	69	-9
4	300	288	16
5	190	181	11
6	237	240	-3
7	-38	28	-11
8	89	107	-15
9	92	85	4
10	-38	41	-8
11	47	44	0

h 5 -1

0	176	173	4
1	32	31	0
2	52	57	-2
3	243	235	11
4	450	443	11
5	189	176	18
6	117	109	8
7	54	80	-13
8	94	104	-9
9	94	94	0
10	170	181	-15
11	130	127	2

h 5 0

1	166	154	19
2	223	212	14
3	36	67	-15
4	114	97	18
5	158	151	9
6	182	185	-5
7	22	42	-6
8	170	155	20
9	122	120	2

10	-49	48	-18
11	12	53	-8

h	5	1	
0	183	179	6
1	52	52	0
2	33	71	-18
3	254	231	31
4	433	434	-1
5	184	172	19
6	95	102	-5
7	92	84	6
8	104	119	-15
9	25	92	-25
10	151	178	-37
11	116	124	-8

h	5	2	
1	171	148	35
2	200	181	23
3	89	57	21
4	312	301	16
5	172	175	-4
6	252	248	3
7	37	27	1
8	119	111	8
9	80	85	-3
10	25	41	-4
11	7	36	-4

h	5	3	
0	381	371	15
1	141	142	-1
2	248	237	14
3	254	250	5
4	306	300	9
5	126	115	13
6	95	102	-6
7	138	138	0
8	109	126	-18
9	76	76	0
10	113	139	-28
11	113	122	-6

h	5	4	
1	216	209	10
2	295	308	-18
3	93	87	6
4	-65	35	-18
5	119	125	-6
6	78	90	-10
7	72	55	10
8	138	145	-9
9	196	211	-18
10	130	153	-27

h	5	5	
0	258	251	8
1	177	173	5
2	120	125	-6
3	128	118	12
4	158	156	1
5	79	98	-13
6	172	182	-15
7	172	177	-6
8	141	149	-10
9	98	106	-7

h	5	6	
1	199	198	1
2	307	318	-16
3	75	56	12
4	135	155	-28
5	146	146	0
6	60	60	0
7	-29	39	-9
8	50	60	-4

h	5	7	
0	255	260	-7
1	176	170	8
2	101	94	6
3	78	69	6
4	86	89	-2
5	-28	8	-3
6	176	186	-14
7	220	231	-16

h	5	8	
1	88	88	0
2	174	170	5
3	80	74	4
4	65	79	-6
5	77	75	1

h	5	9	
0	286	300	-19
1	139	148	-10
2	59	69	-3

h	6	-6	
0	177	179	-3
1	70	59	4
2	70	55	7
3	139	131	8

h	6	-5	
1	-22	58	-10
2	77	85	-5
3	142	126	18
4	63	77	-6
5	127	102	23

h	6	-4	
0	97	121	-18
1	106	120	-13
2	78	60	8
3	122	115	6
4	123	107	14
5	99	81	13
6	119	101	15

h	6	-3	
1	120	108	12
2	145	127	20
3	73	41	13
4	50	66	-5
5	114	105	8
6	100	94	4
7	-61	2	-12

h	6	-2	
0	130	130	0
1	111	106	5
2	57	46	5
3	116	102	12
4	87	78	6
5	18	35	-3
6	-52	80	-22
7	168	141	31

h	6	-1	
1	130	104	26
2	169	159	14
3	173	175	-3
4	150	152	-2
5	264	250	15
6	97	78	11
7	38	79	-16
8	99	92	4

h	6	0	
0	621	599	29
1	347	318	39
2	164	176	-19
3	258	257	1
4	93	76	13
5	100	82	15
6	57	68	-6
7	175	177	-3
8	83	125	-31

h	6	1	
1	114	101	12
2	161	169	-11
3	179	188	-13
4	148	164	-22
5	245	273	-39
6	79	85	-3
7	70	77	-3
8	92	98	-4

h	6	2	
0	129	126	4
1	83	99	-14
2	70	53	11
3	109	132	-25
4	89	93	-3
5	36	42	-1
6	95	78	14
7	129	134	-5

h	6	3	
1	109	106	3
2	141	127	17
3	44	25	4
4	88	66	10
5	97	102	-3
6	91	95	-3
7	45	1	6

h	6	4	
0	122	132	-11
1	108	109	0
2	92	67	19
3	126	123	3
4	113	115	-2
5	58	88	-17
6	29	90	-27

h	6	5	
1	74	58	10
2	-33	78	-23
3	122	123	0
4	16	81	-19
5	108	101	5

h	6	6	
0	138	150	-14
1	43	48	-1
2	-51	52	-16
3	139	134	5

I-1147-M65

Table S6E. Observed and Calculated Structure Factors for 4′-Methoxy-N-methyl-4-stilbazolium Chloride

The columns contain, in order, h, $10F_{obs}$, $10F_{calc}$ and $10\left(\frac{F^2_{obs}-F^2_{calc}}{\sigma F^2_{obs}}\right)$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

I-1147-m66

h	0	0	
2	827	879	-58
4	1208	1240	-24
6	413	409	9
8	82	82	-3
10	88	83	20
12	134	116	50
14	88	77	46
16	93	89	10
18	67	51	33

h	1	0	
1	75	50	154
2	64	70	-41
3	21	19	7
4	22	9	50
5	60	63	-30
6	73	69	29
7	82	87	-29
8	150	148	10
9	-11	19	-20
10	109	113	-20
11	20	28	-6
12	110	112	-8
13	-11	10	-11
14	106	103	12
15	23	23	-1
16	62	54	41
17	4	14	-7
18	36	28	13
19	19	7	9

h	2	0	
0	2521	2528	-2
1	539	541	-2
2	2042	2022	10
3	533	523	21
4	424	425	-3
5	296	307	-37
6	469	462	17
7	124	121	15
8	447	434	30
9	129	130	-5
10	212	216	-16
11	16	12	3
12	208	205	9
13	82	89	-44
14	37	46	-41
15	-26	8	-19
16	36	42	-27
17	7	16	-6
18	17	17	0

h	3	0	
1	2	9	-3
2	41	47	-45
3	75	81	-40
4	16	38	-49
5	41	35	37
6	43	50	-50
7	145	146	-4
8	124	129	-21
9	27	27	0
10	173	171	8
11	64	69	-38
12	15	8	7
13	4	1	0
14	121	119	4
15	59	53	30
16	30	28	2
17	5	20	-10

h	4	0	
0	1244	1231	11
1	464	459	12
2	455	445	22
3	284	293	-28
4	401	394	18
5	345	356	-32
6	108	105	14
7	142	147	-22
8	69	68	7
9	148	142	22
10	11	25	-23
11	24	3	28
12	92	97	-30
13	123	116	30
14	15	13	2
15	-22	4	-15
16	44	45	0

h	5	0	
1	-16	1	-8
2	18	18	0
3	49	53	-19
4	40	33	30
5	26	30	-10
6	9	17	-6
7	80	77	23
8	19	14	7
9	19	14	8
10	-11	5	-4
11	50	39	45
12	65	65	0
13	16	14	1
14	34	33	2

h	6	0	
0	344	362	-51
1	254	257	-9
2	146	146	0
3	121	122	-5
4	167	179	-41
5	194	197	-8
6	-10	7	-6
7	59	59	0
8	16	2	10
9	58	51	18
10	21	5	12
11	21	10	10

h	7	0	
1	-19	7	-10
2	34	15	28
3	-12	15	-10
4	-15	8	-7
5	1	18	-8
6	4	3	0
7	46	43	7

h	0	1	
2	508	495	28
4	1240	1256	-13
6	1020	1016	4
8	213	217	-17
10	380	369	29
12	289	292	-10
14	25	30	-12
16	75	76	-4
18	33	18	23

h	1	1	
0	354	334	68
1	41	32	119
2	87	91	-28
3	88	90	-15
4	1025	1022	4
5	189	188	2
6	125	125	0
7	100	102	-16
8	613	609	9
9	69	69	2
10	176	176	0
11	57	54	22
12	251	261	-42
13	44	43	6
14	134	131	15
15	-10	7	-11
16	13	10	4
17	-21	1	-15
18	68	65	13
19	6	8	-1

h	2	1	
2	1081	1039	48
3	445	442	5
4	131	141	-67
5	315	316	-6
6	221	217	20
7	119	118	2
8	472	462	25
9	61	60	10
10	204	200	15
11	80	77	18
12	88	87	3
13	32	32	0
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17	23	19	6
18	32	23	20

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8	248	252	-16
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12	141	137	24
13	81	79	18
14	90	79	78
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6	78	79	-5
7	123	122	3
8	88	92	-33
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12	70	77	-36
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12	227	226	1
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16	122	131	-37
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6	78	79	-3
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3	214	221	-37
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6	174	175	-5
7	89	93	-29
8	199	205	-27
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5	89	84	36
6	142	143	-10
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5	134	135	-5
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13	90	91	-8
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15	34	32	7
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7	73	70	26
8	160	157	10
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12	26	27	-1
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7	61	66	-20
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14	181	185	-15
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8	89	88	7
9	13	8	7
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16	91	101	-53
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7	117	119	-12
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9	67	72	-46
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14	54	54	-5
15	27	30	-6
16	10	13	-2

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12	33	31	3
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7	47	49	-5
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3	138	139	-1
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5	93	96	-20
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8	112	113	-7
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7	77	79	-17
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12	191	191	0
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15	-7	4	-3
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h 2 7

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h 0 8

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h 1 8

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8	247	246	5
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11	7	13	-4
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13	18	29	-15
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h 3 8

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h 4 8

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7	118	116	13
8	98	99	-4
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h 5 8

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h 2 9

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3	46	44	14
4	53	53	0
5	56	57	-3
6	79	78	11
7	40	42	-8
8	83	84	-8
9	-11	18	-15
10	42	41	3
11	23	29	-12
12	122	122	0
13	35	38	-7
14	31	20	24

h 3 9

0	97	100	-16
1	98	96	8
2	27	32	-25
3	85	87	-14
4	65	66	-9
5	65	64	9
6	88	89	-1
7	70	71	-11
8	140	136	21
9	57	58	-3
10	115	121	-35
11	49	50	-5
12	89	88	8
13	30	22	16

h 4 9

1	64	63	7
2	13	17	-6
3	41	36	28
4	12	14	-3
5	53	46	46
6	43	44	-7
7	69	61	50
8	36	39	-9
9	28	16	20
10	22	23	-2
11	-12	11	-11

h 5 9

0	118	119	-9
1	93	92	6
2	86	85	8
3	91	87	17
4	67	65	6
5	74	67	31
6	53	45	26
7	54	55	-4
8	31	36	-11

h 6 9

1	21	32	-20
2	-13	18	-19

h 0 10

0	73	63	61
2	124	123	6
4	245	247	-8
6	143	146	-9
8	128	127	4

10	211	220	-31
12	38	39	-3
14	44	63	-49

h 1 10

1	44	49	-34
2	54	54	0
3	71	71	-4
4	112	116	-24
5	81	79	18
6	27	29	-7
7	43	40	15
8	66	64	18
9	-12	8	-7
10	101	101	-1
11	12	8	4
12	33	35	-4
13	12	13	0
14	70	67	13

h 2 10

0	221	227	-27
1	34	37	-12
2	204	210	-27
3	79	78	8
4	210	208	9
5	48	53	-35
6	57	57	2
7	54	55	-5
8	29	37	-40
9	56	58	-14
10	121	121	-2
11	35	33	7
12	34	33	2
13	19	21	-3

h 3 10

1	49	48	7
2	48	50	-9
3	42	36	39
4	87	84	19
5	26	30	-12
6	68	67	3
7	12	6	6
8	9	10	0
9	27	29	-5
10	45	42	11
11	19	24	-9
12	37	41	-8

h 4 10

0	71	72	-9
1	77	78	-11
2	78	75	18
3	133	132	4
4	93	88	34
5	100	95	29
6	52	47	17
7	35	40	-14
8	42	37	12
9	79	78	2
10	77	81	-17

h 5 10

1	42	42	0
2	32	36	-9
3	23	23	-1
4	48	54	-20
5	24	28	-7
6	30	22	15

h 0 11

2	246	252	-20
4	197	205	-30
6	148	149	-5
8	-4	35	-29
10	19	29	-12
12	-10	4	-4

h 1 11

0	258	254	14
1	127	126	7
2	290	282	29
3	75	76	-8
4	161	161	1
5	37	37	2
6	122	120	11
7	39	31	41
8	130	131	-4
9	14	12	1
10	43	48	-18
11	13	13	0
12	47	40	20
13	15	9	6

h 2 11

1	87	87	-6
2	188	191	-13
3	36	36	0
4	162	166	-17
5	16	22	-15
6	89	92	-24
7	25	27	-4
8	47	45	13
9	14	18	-5
10	38	36	5
11	20	5	17
12	27	26	3

h 3 11

0	172	166	27
1	54	55	-8
2	214	210	18
3	42	38	22
4	106	103	14
5	60	53	40
6	115	111	21
7	75	75	1
8	108	102	32
9	55	53	7
10	43	41	7

h 4 11

1	105	103	11
2	91	94	-14
3	17	16	0
4	79	79	0
5	44	40	9
6	54	56	-7
7	46	40	16
8	19	10	11

h 5 11

0	104	106	-7
1	64	60	14
2	96	92	16
3	39	36	6

h 0 12

0	264	266	-6
2	140	140	0
4	192	194	-9
6	235	236	-5
8	86	85	4
10	47	48	-1

h 1 12

1	16	15	1
2	3	19	-18
3	15	22	-12
4	16	27	-27
5	49	46	17
6	104	103	1
7	43	46	-17
8	43	41	4
9	16	10	7
10	34	21	29
11	23	21	4

h 2 12

0	144	142	9
1	38	41	-18
2	64	55	67
3	19	14	9
4	131	129	10
5	39	38	5
6	167	167	1
7	73	71	7
8	94	94	-2
9	48	45	8
10	52	58	-20

h 3 12

1	24	28	-10
2	30	33	-7
3	41	42	-2
4	51	50	3
5	2	8	-2
6	52	57	-17
7	49	50	-5
8	23	31	-16

h 4 12

0	84	80	17
1	91	88	14
2	31	30	1
3	64	60	15
4	79	74	23
5	47	46	2

h 0 13

2	75	79	-21
4	103	107	-17
6	25	18	9
8	40	33	14

h 1 13

0	66	68	-16
1	-16	4	-13
2	89	86	21
3	-18	11	-20
4	116	116	0
5	-3	8	-3
6	81	81	0
7	23	13	15
8	69	73	-18
9	21	12	11

h 2 13

1	42	39	11
2	57	56	5
3	34	36	-5
4	95	93	8
5	31	34	-6
6	30	29	2
7	30	21	18
8	-16	2	-10

h 3 13

0	88	81	34
1	50	49	2
2	91	88	15
3	68	64	15
4	80	76	16
5	55	53	8
6	24	41	-27

h 0 14

0	101	88	47
2	105	108	-11
4	63	67	-12
6	45	58	-34

h 1 14

1	-18	6	-14
2	13	8	3
3	20	14	7
4	14	12	1
5	13	12	1
6	37	43	-18

h 2 14

0	64	61	12
1	59	58	5
2	87	82	25
3	52	45	22
4	71	72	-1